

10590585.trn

Connecting via Winsock to STN

Welcome to STN International! Enter x:X

LOGINID:SSPTADK01625

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	AUG 10	Time limit for inactive STN sessions doubles to 40 minutes
NEWS	3	AUG 18	COMPENDEX indexing changed for the Corporate Source (CS) field
NEWS	4	AUG 24	ENCOMPLIT/ENCOMPLIT2 reloaded and enhanced
NEWS	5	AUG 24	CA/CAPLUS enhanced with legal status information for U.S. patents
NEWS	6	SEP 09	50 Millionth Unique Chemical Substance Recorded in CAS REGISTRY
NEWS	7	SEP 11	WPIDS, WPINDEX, and WPIX now include Japanese FTERM thesaurus
NEWS	8	OCT 21	Derwent World Patents Index Coverage of Indian and Taiwanese Content Expanded
NEWS	9	OCT 21	Derwent World Patents Index enhanced with human translated claims for Chinese Applications and Utility Models
NEWS	10	OCT 27	Free display of legal status information in CA/CAPLUS, USPTAFULL, and USPAT2 in the month of November.
NEWS	11	NOV 23	Addition of SCAN format to selected STN databases
NEWS	12	NOV 23	Annual Reload of IFI Databases

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:40:11 ON 23 NOV 2009

=> file reg

FILE 'REGISTRY' ENTERED AT 11:40:27 ON 23 NOV 2009

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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 22 NOV 2009 HIGHEST RN 1193309-59-9
DICTIONARY FILE UPDATES: 22 NOV 2009 HIGHEST RN 1193309-59-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

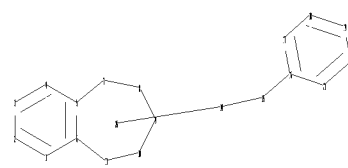
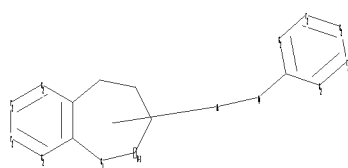
REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10590585-coresearch.str

10590585.trn



```
chain nodes :  
14 15  
ring nodes :  
1 2 3 4 5 6 7 8 9 10 11 16 17 18 19 20 21  
chain bonds :  
14-15 15-16  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-11 7-8 8-9 9-10 10-11 16-17 16-21 17-18  
18-19 19-20 20-21  
exact/norm bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-11 7-8 8-9 9-10 10-11 14-15 15-16 16-17  
16-21 17-18 18-19 19-20 20-21
```

G1:C,O,S,N

G2:C,N

10590585.trn

Match level :

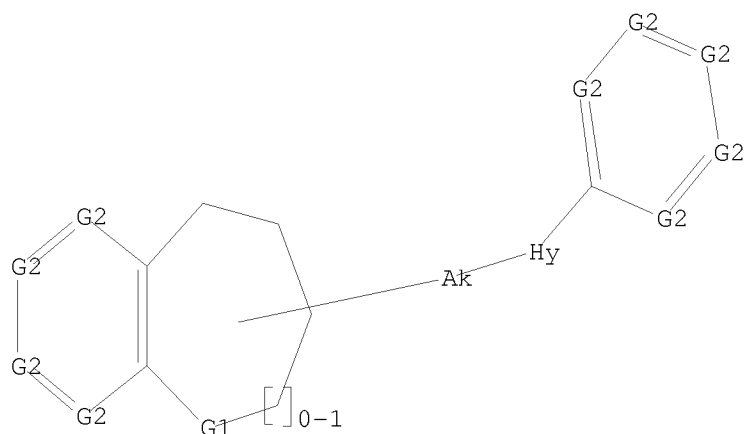
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
26:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 C,O,S,N

G2 C,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 11:40:44 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2184605 TO ITERATE

0.1% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 43622645 TO 43761555
PROJECTED ANSWERS: 19864 TO 23828

L2 1 SEA SSS SAM L1

=>

Connecting via Winsock to STN

Welcome to STN International! Enter x:X

10590585.trn

LOGINID:SSPTADKO1625

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	AUG 10	Time limit for inactive STN sessions doubles to 40 minutes
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NEWS	10	NOV 23	Addition of SCAN format to selected STN databases
NEWS	11	NOV 23	Annual Reload of IFI Databases
NEWS	12	DEC 01	FRFULL Content and Search Enhancements
NEWS	13	DEC 01	DGENE, USGENE, and PCTGEN: new percent identity feature for sorting BLAST answer sets
NEWS	14	DEC 02	Derwent World Patent Index: Japanese FI-TERM thesaurus added
NEWS	15	DEC 02	PCTGEN enhanced with patent family and legal status display data from INPADOCDB
NEWS	16	DEC 02	USGENE: Enhanced coverage of bibliographic and sequence information
NEWS	17	DEC 21	New Indicator Identifies Multiple Basic Patent Records Containing Equivalent Chemical Indexing in CA/CAPLUS
NEWS	18	JAN 12	Match STN Content and Features to Your Information Needs, Quickly and Conveniently
NEWS	19	JAN 25	Annual Reload of MEDLINE database
NEWS	20	FEB 16	STN Express Maintenance Release, Version 8.4.2, Is Now Available for Download
NEWS	21	FEB 16	Derwent World Patents Index (DWPI) Revises Indexing of Author Abstracts
NEWS	22	FEB 16	New FASTA Display Formats Added to USGENE and PCTGEN
NEWS	23	FEB 16	INPADOCDB and INPAFAMDB Enriched with New Content and Features
NEWS	24	FEB 16	INSPEC Adding Its Own IPC codes and Author's E-mail Addresses

NEWS EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2,
AND CURRENT DISCOVER FILE IS DATED 15 JANUARY 2010.

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NEWS LOGIN Welcome Banner and News Items

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:13:41 ON 23 FEB 2010

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

FILE 'REGISTRY' ENTERED AT 11:14:17 ON 23 FEB 2010

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STRUCTURE FILE UPDATES: 21 FEB 2010 HIGHEST RN 1206966-88-2

DICTIONARY FILE UPDATES: 21 FEB 2010 HIGHEST RN 1206966-88-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

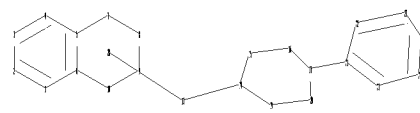
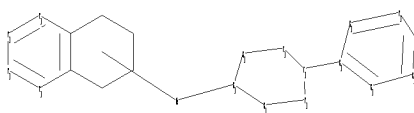
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10590585-9.str

10590585.trn



```
chain nodes :
13
ring nodes :
1 2 3 4 5 6 7 8 9 10 14 15 16 17 19 20 21 22 23 24 26 27
chain bonds :
13-14 17-21
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 14-15 14-19 15-16 16-17
17-20 19-20 21-22 21-23 22-27 23-24 24-26 26-27
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 9-10 13-14 14-15 14-19 15-16 16-17
17-20 17-21 19-20 21-22 21-23 22-27 23-24 24-26 26-27
exact bonds :
7-8 8-9
```

G1:C,N

```
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom 26:Atom 27:Atom 28:CLASS
```

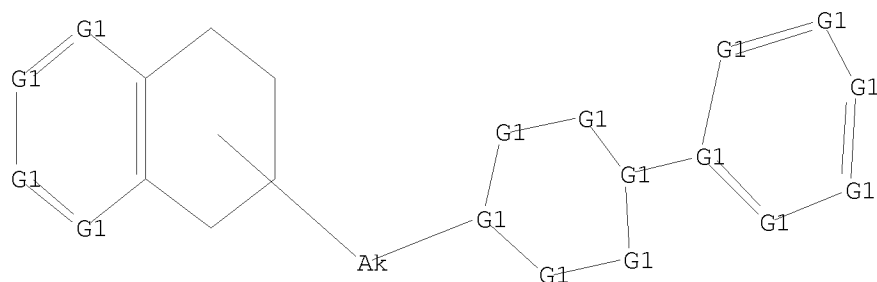
10590585.trn

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 C,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 11:14:37 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 536104 TO ITERATE

0.4% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 10680258 TO 10763902

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

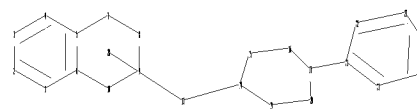
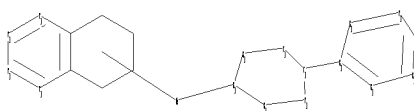
=> screen 1841 AND 1992

L3 SCREEN CREATED

=>

Uploading C:\Program Files\Stnexp\Queries\10590585-8.str

10590585.trn



```
chain nodes :
13
ring nodes :
1 2 3 4 5 6 7 8 9 10 14 15 16 17 19 20 21 22 23 24 26 27
chain bonds :
13-14 17-21
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 14-15 14-19 15-16 16-17
17-20 19-20 21-22 21-23 22-27 23-24 24-26 26-27
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 9-10 13-14 14-15 14-19 15-16 16-17
17-20 17-21 19-20 21-22 21-23 22-27 23-24 24-26 26-27
exact bonds :
7-8 8-9
```

G1:C,N

```
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom 26:Atom 27:Atom 28:CLASS
```

10590585.trn

L4 STRUCTURE UPLOADED

=> que L4 AND L3

L5 QUE L4 AND L3

=>Testing the current file.... screen

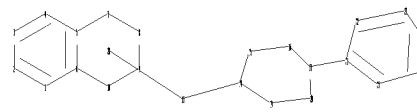
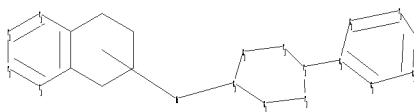
ENTER SCREEN EXPRESSION OR (END):end

=> screen 1840 AND 1992

L6 SCREEN CREATED

=>

Uploading C:\Program Files\Stnexp\Queries\10590585-5.str



chain nodes :

13

ring nodes :

1 2 3 4 5 6 7 8 9 10 14 15 16 17 19 20 21 22 23 24 26 27

chain bonds :

13-14 17-21

10590585.trn

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 14-15 14-19 15-16 16-17
17-20 19-20 21-22 21-23 22-27 23-24 24-26 26-27

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 9-10 13-14 14-15 16-17 17-20 17-21
21-22 21-23 22-27 23-24 24-26 26-27

exact bonds :

7-8 8-9 14-19 15-16 19-20

G1:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom 26:Atom 27:Atom 28:CLASS

L7 STRUCTURE UPLOADED

=> que L7 AND L6

L8 QUE L7 AND L6

=> s 18

SAMPLE SEARCH INITIATED 11:16:27 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 419348 TO ITERATE

0.5% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 8349557 TO 8424363
PROJECTED ANSWERS: 0 TO 0

L9 0 SEA SSS SAM L7 AND L6

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

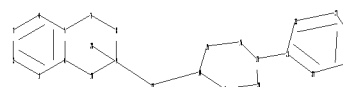
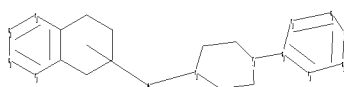
=> screen 1992 AND 1840

L10 SCREEN CREATED

=>

Uploading C:\Program Files\Stnexp\Queries\10590585-999.str

10590585.trn



```
chain nodes :
13
ring nodes :
1  2  3  4  5  6  7  8  9  10  14  15  16  17  19  20  21  22  23  24  26  27
chain bonds :
13-14  17-21
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10  14-15  14-19  15-16  16-17
17-20  19-20  21-22  21-23  22-27  23-24  24-26  26-27
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  9-10  13-14  16-17  17-20  17-21  21-22
21-23  22-27  23-24  24-26  26-27
exact bonds :
7-8  8-9  14-15  14-19  15-16  19-20
```

G1:C,N

```
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom 26:Atom 27:Atom 28:CLASS
```

L11 STRUCTURE UPLOADED

=> que L11 AND L10

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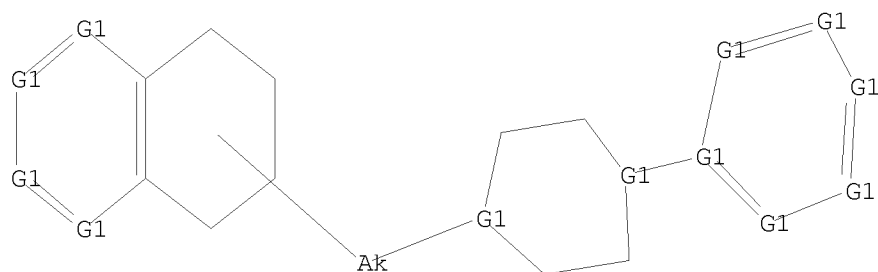
L12 QUE L11 AND L10

=> d l12

L12 HAS NO ANSWERS

L10 SCR 1992 AND 1840

L11 STR



G1 C,N

Structure attributes must be viewed using STN Express query preparation.

L12 QUE ABB=ON PLU=ON L11 AND L10

=> s l12

SAMPLE SEARCH INITIATED 11:18:04 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 312257 TO ITERATE

0.6% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 6212540 TO 6277740

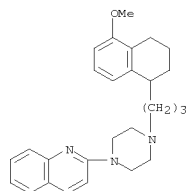
PROJECTED ANSWERS: 2373 TO 3871

L13 1 SEA SSS SAM L11 AND L10

=> d scan

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L13 1 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Quinoline,
2-[4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]-1-
piperazinyl]-, hydrochloride (1:2)
MF C27 H33 N3 O . 2 Cl H



● 2 HCl

ALL ANSWERS HAVE BEEN SCANNED

10590585.trn

=> s piperidine/cn

L14 1 PIPERIDINE/CN

=> d rsd

10590585.trn

L14 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2010 ACS on STN

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C5N	INC5	6	C5N	46.156.1	1

10590585.trn

=> s 46.156.1/rid

L15 2737850 46.156.1/RID

=> s piperazine

L16 547740 PIPERAZINE

=> s piperazine/cn

L17 1 PIPERAZINE/CN

=> d rsd

10590585.trn

L17 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2010 ACS on STN

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C4N2	INC2NC2	16	C4N2	146.383.1	1

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=> s 46.383.1/rid

L18 1597508 46.383.1/RID

=> d his

(FILE 'HOME' ENTERED AT 11:13:41 ON 23 FEB 2010)

FILE 'REGISTRY' ENTERED AT 11:14:17 ON 23 FEB 2010

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 SCREEN 1841 AND 1992
L4 STRUCTURE UPLOADED
L5 QUE L4 AND L3
L6 SCREEN 1840 AND 1992
L7 STRUCTURE UPLOADED
L8 QUE L7 AND L6
L9 0 S L8
L10 SCREEN 1992 AND 1840
L11 STRUCTURE UPLOADED
L12 QUE L11 AND L10
L13 1 S L12
L14 1 S PIPERIDINE/CN
L15 2737850 S 46.156.1/RID
L16 547740 S PIPERAZINE
L17 1 S PIPERAZINE/CN
L18 1597508 S 46.383.1/RID

=> s l18 and l15

L19 90686 L18 AND L15

=> s l18 or l15

SYSTEM LIMITS EXCEEDED - SEARCH ENDED

The search profile you entered was too complex or gave too many answers. Simplify or subdivide the query and try again. If you have exceeded the answer limit, enter DELETE HISTORY at an arrow prompt (=>) to remove all previous answers sets and begin at L1. Use the SAVE command to store any important profiles or answer sets before using DELETE HISTORY.

=> d his

(FILE 'HOME' ENTERED AT 11:13:41 ON 23 FEB 2010)

FILE 'REGISTRY' ENTERED AT 11:14:17 ON 23 FEB 2010

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 SCREEN 1841 AND 1992
L4 STRUCTURE UPLOADED
L5 QUE L4 AND L3
L6 SCREEN 1840 AND 1992
L7 STRUCTURE UPLOADED
L8 QUE L7 AND L6
L9 0 S L8
L10 SCREEN 1992 AND 1840
L11 STRUCTURE UPLOADED

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L12 QUE L11 AND L10
L13 1 S L12
L14 1 S PIPERIDINE/CN
L15 2737850 S 46.156.1/RID
L16 547740 S PIPERAZINE
L17 1 S PIPERAZINE/CN
L18 1597508 S 46.383.1/RID
L19 90686 S L18 AND L15

=> s sub=l15 sam l12

SAMPLE SUBSET SEARCH INITIATED 11:21:21 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED - 45000 TO ITERATE

4.4% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET): ONLINE **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET): 887323 TO 912677
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 0 TO 0

L20 0 SEA SUB=L15 SSS SAM L11 AND L10

=> s sub=l15 full l12

FULL SUBSET SEARCH INITIATED 11:21:30 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 905986 TO ITERATE

98.7% PROCESSED 893804 ITERATIONS 394 ANSWERS
100.0% PROCESSED 905986 ITERATIONS 394 ANSWERS
SEARCH TIME: 00.00.18

L21 394 SEA SUB=L15 SSS FUL L11 AND L10

=> s sub=l19 full l12

FULL SUBSET SEARCH INITIATED 11:22:02 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 23135 TO ITERATE

100.0% PROCESSED 23135 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L22 0 SEA SUB=L19 SSS FUL L11 AND L10

=> s sub=l18 full l12

FULL SUBSET SEARCH INITIATED 11:22:20 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 281857 TO ITERATE

100.0% PROCESSED 281857 ITERATIONS 372 ANSWERS
SEARCH TIME: 00.00.06

L23 372 SEA SUB=L18 SSS FUL L11 AND L10

=> s l21 or l23

L24 766 L21 OR L23

10590585.trn

=> file caplus

FILE 'CAPLUS' ENTERED AT 11:22:38 ON 23 FEB 2010
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FILE COVERS 1907 - 23 Feb 2010 VOL 152 ISS 9
FILE LAST UPDATED: 22 Feb 2010 (20100222/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2009

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 124
L25 96 L24

=> file reg

FILE 'REGISTRY' ENTERED AT 11:22:47 ON 23 FEB 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 FEB 2010 HIGHEST RN 1206966-88-2
DICTIONARY FILE UPDATES: 21 FEB 2010 HIGHEST RN 1206966-88-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and

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predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> rea rn l25

READ COMMAND IS VALID ONLY IN THE MAIL FILE

Mail functions are available only in the mail file. For an explanation of how to use the electronic mail service, enter "HELP MAIL". For more information, enter "HELP READ".

=> tra rn l25

L26 TRANSFER L25 1- RN : 21131 TERMS

SEARCH OF L26 IS APPROXIMATELY 43% COMPLETE

SEARCH OF L26 IS APPROXIMATELY 86% COMPLETE

L27 21131 L26

=> d his

(FILE 'HOME' ENTERED AT 11:13:41 ON 23 FEB 2010)

FILE 'REGISTRY' ENTERED AT 11:14:17 ON 23 FEB 2010

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 SCREEN 1841 AND 1992
L4 STRUCTURE UPLOADED
L5 QUE L4 AND L3
L6 SCREEN 1840 AND 1992
L7 STRUCTURE UPLOADED
L8 QUE L7 AND L6
L9 0 S L8
L10 SCREEN 1992 AND 1840
L11 STRUCTURE UPLOADED
L12 QUE L11 AND L10
L13 1 S L12
L14 1 S PIPERIDINE/CN
L15 2737850 S 46.156.1/RID
L16 547740 S PIPERAZINE
L17 1 S PIPERAZINE/CN
L18 1597508 S 46.383.1/RID
L19 90686 S L18 AND L15
L20 0 S SAM L12 SUB=L15
L21 394 S FULL L12 SUB=L15
L22 0 S FULL L12 SUB=L19
L23 372 S FULL L12 SUB=L18
L24 766 S L21 OR L23

FILE 'CAPLUS' ENTERED AT 11:22:38 ON 23 FEB 2010

L25 96 S L24

FILE 'REGISTRY' ENTERED AT 11:22:47 ON 23 FEB 2010

FILE 'CAPLUS' ENTERED AT 11:22:56 ON 23 FEB 2010

L26 TRA L25 1- RN : 21131 TERMS

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FILE 'REGISTRY' ENTERED AT 11:23:05 ON 23 FEB 2010
L27 21131 SEA L26

=> s 124 not 127
L28 160 L24 NOT L27

=> help dfields

The display fields that you may use to display REGISTRY File records are listed below. You may use any of the SUBSTANCE INFORMATION FIELD CODES or PROPERTY FIELD CODES with the DISPLAY and PRINT commands. You may also use any of the CA DOCUMENT REFERENCE FIELD CODES OR PREDEFINED FORMATS, but these must always be combined with one of the Substance Information fields or formats. The fields appear in the order you request them.

The Component Number (CM) field code appears in records for multicomponent substances but is not a custom display field.

Substance Information Display Field Codes

AF	Alternate Molecular Formula
AR	Alternate CAS Registry Number
CCI	Component Class Identifier
CCN	Condensed Chemical Name (all names)
CI	Class Identifier
CIL	Component Isotope at Unknown Location
CMF	Component Molecular Formula
CN	Chemical Name (up to 50)
COMP	Composition
CRN	Component CAS Registry Number
DEF	Definition
DR	Deleted CAS Registry Number
ED	Entry Date
ENTE	Editor Note
FCN	All Chemical Names
FS	File Segment
IL	Isotope at Unknown Location
IN	CA Index Name
LC	CAS Registry Number Locator
MF	Molecular Formula
PCT	Polymer Class Term
PR	Preferred CAS Registry Number
REF	Number of References in CAlplus and CA files and the number of references in CA for the non-specific derivatives
RN	CAS Registry Number
RR	Replacing Registry Number
RSD	Ring System Data
SCN	Short Chemical Name (IN and OTHER NAMES)
SR	Source of Registration
SRSD	Short Ring System Data
STR	Structure Diagram with stereo bond and R/S/Z/E designations, if available

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STF	Flat Structure Diagram (no stereo bonds)
STS	Structure Diagram with stereo bonds, if available

Biosequence Field Codes

NA	Nucleic Acid
NTE	Note
PNTE	Patent Annotation
SEQ	Sequence (1-letter amino acid codes)
SEQ3	Sequence (3-letter amino acid codes)
SQL	Sequence Length

Property Field Codes

BCF	Bioconcentration Factor
BP	Boiling Point
DEN	Density
ECND	Electric Conductivity
ECON	Electric Conductance
ERES	Electric Resistance
EREST	Electric Resistivity
ETAG	Experimental Property Tags
FP	Flash Point
FRB	Freely Rotable Bonds
HAC	H acceptors
HD	H donors
HDAS	H Donor/Acceptor Sum
HVAP	Enthalpy of Vaporization
ISLB.MASS	Mass Intrinsic Solubility
KOC	Organic Carbon Adsorption Coefficient
LD50	Median Lethal Dose
LOGD	logD
LOGP	logP
MM	Magnetic Moment
MP	Melting Point
MW	Molecular Weight
ORP	Optical Rotatory Power
PKA	pKa
PSA	Polar Surface Area
RI	Refractive Index
SLB.MASS	Mass Solubility
SLB.MOL	Molar Solubility
SPEC	Spectra
SPEC.C13NMR	Carbon-13 NMR Spectra
SPEC.IR	IR Absorption Spectra
SPEC.MASS	Mass Spectra
SPEC.H1NMR	Proton NMR Spectra
TG	Glass Transition Temperature
TS	Tensile Strength
VP	Vapor Pressure

Caplus Super Roles and Document Type Display Field codes

DT.CA	Caplus document type
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RL	CAPLUS super roles
RL.NP	CAPLUS super roles from non-patents
RL.P	CAPLUS super roles from patents
RLD (RL.D)	CAPLUS super roles for non-specific derivatives
RLD. NP	CAPLUS super roles for non-specific derivatives from non-patents
RLD.P	CAPLUS super roles for non-specific derivatives from patents
RLS	CAPLUS super roles for the specific substance and its non-specific derivatives

For more information on display options, enter HELP FORMAT at an arrow prompt (=>). To find out about extracting search terms from display fields, enter HELP SELECT and HELP ANALYZE. For a list of fields that may be used with the ANALYZE and SELECT commands, enter HELP EFIELDS.

=> d his

(FILE 'HOME' ENTERED AT 11:13:41 ON 23 FEB 2010)

FILE 'REGISTRY' ENTERED AT 11:14:17 ON 23 FEB 2010

L1	STRUCTURE UPLOADED
L2	0 S L1
L3	SCREEN 1841 AND 1992
L4	STRUCTURE UPLOADED
L5	QUE L4 AND L3
L6	SCREEN 1840 AND 1992
L7	STRUCTURE UPLOADED
L8	QUE L7 AND L6
L9	0 S L8
L10	SCREEN 1992 AND 1840
L11	STRUCTURE UPLOADED
L12	QUE L11 AND L10
L13	1 S L12
L14	1 S PIPERIDINE/CN
L15	2737850 S 46.156.1/RID
L16	547740 S PIPERAZINE
L17	1 S PIPERAZINE/CN
L18	1597508 S 46.383.1/RID
L19	90686 S L18 AND L15
L20	0 S SAM L12 SUB=L15
L21	394 S FULL L12 SUB=L15
L22	0 S FULL L12 SUB=L19
L23	372 S FULL L12 SUB=L18
L24	766 S L21 OR L23

FILE 'CAPLUS' ENTERED AT 11:22:38 ON 23 FEB 2010

L25 96 S L24

FILE 'REGISTRY' ENTERED AT 11:22:47 ON 23 FEB 2010

FILE 'CAPLUS' ENTERED AT 11:22:56 ON 23 FEB 2010

L26 TRA L25 1- RN : 21131 TERMS

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FILE 'REGISTRY' ENTERED AT 11:23:05 ON 23 FEB 2010

L27 21131 SEA L26
L28 160 S L24 NOT L27

=> analyze l28
ENTER ANSWER NUMBER OR RANGE (1-):1-
ENTER DISPLAY CODE (CHEM) OR ?:lc
L29 ANALYZE L28 1- LC : 2 TERMS

=> d l29
L29 ANALYZE L28 1- LC : 2 TERMS

TERM #	# OCC	# DOC	% DOC	LC
1	40	40	25.00	CHEMCATS
2	1	1	0.62	BEILSTEIN

***** END OF L29***

=> s l28 and chemcats/lc
10783402 CHEMCATS/LC
L30 40 L28 AND CHEMCATS/LC

=> s l28 and beilstein/lc
4362486 BEILSTEIN/LC
L31 1 L28 AND BEILSTEIN/LC

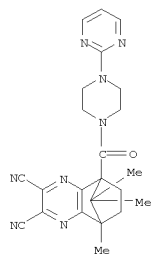
=> s l30 or l31
L32 41 L30 OR L31

=> s l32 and ed<=2005
84720038 ED<=2005
(ED<=20059999)
L33 26 L32 AND ED<=2005

=> d l33 str rn cn ed lc so 1-
YOU HAVE REQUESTED DATA FROM 26 ANSWERS - CONTINUE? Y/(N):y

10590585.trn

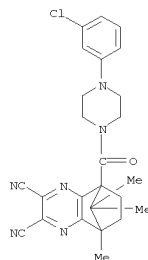
L33 ANSWER 1 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 862262-01-9 REGISTRY
CN INDEX NAME NOT YET ASSIGNED
ED Entered STN: 01 Sep 2005
LC STN Files: CHEMCATS

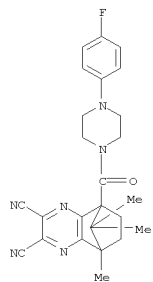
L33 ANSWER 2 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 862261-90-3 REGISTRY
CN INDEX NAME NOT YET ASSIGNED
ED Entered STN: 01 Sep 2005
LC STN Files: CHEMCATS

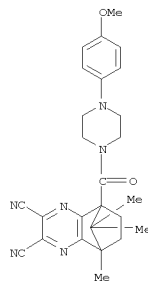
L33 ANSWER 3 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 862257-84-9 REGISTRY
CN INDEX NAME NOT YET ASSIGNED
ED Entered STN: 01 Sep 2005
LC STN Files: CHEMCATS

L33 ANSWER 4 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN

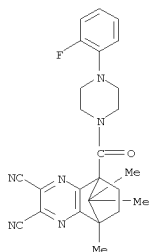


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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CN INDEX NAME NOT YET ASSIGNED
ED Entered STN: 01 Sep 2005
LC STN Files: CHEMCATS

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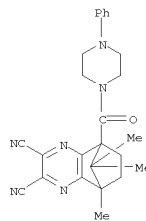
L33 ANSWER 5 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 862257-81-6 REGISTRY
CN INDEX NAME NOT YET ASSIGNED
ED Entered STN: 01 Sep 2005
LC STN Files: CHEMCATS

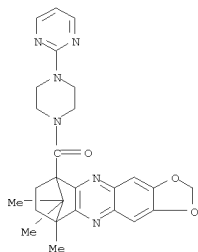
L33 ANSWER 6 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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CN INDEX NAME NOT YET ASSIGNED
ED Entered STN: 01 Sep 2005
LC STN Files: CHEMCATS

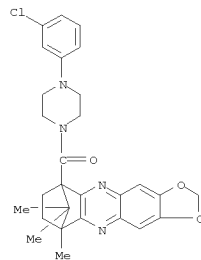
L33 ANSWER 7 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 821812-46-8 REGISTRY
CN Methanone, (8,9-dihydro-9,12,12-trimethyl-6,9-methano-1,3-dioxolo[4,5-b]phenazin-6(7H)-yl)[4-(2-pyrimidinyl)-1-piperazinyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[(8,9-dihydro-9,12,12-trimethyl-6,9-methano-1,3-dioxolo[4,5-b]phenazin-6(7H)-yl)carbonyl]-4-(2-pyrimidinyl)- (9CI)
ED Entered STN: 28 Jan 2005
LC STN Files: CHEMCATS

L33 ANSWER 8 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN

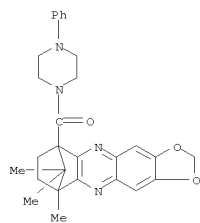


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 821811-34-1 REGISTRY
CN Methanone, [4-(3-chlorophenyl)-1-piperazinyl](8,9-dihydro-9,12,12-trimethyl-6,9-methano-1,3-dioxolo[4,5-b]phenazin-6(7H)-yl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-(3-chlorophenyl)-4-[(8,9-dihydro-9,12,12-trimethyl-6,9-methano-1,3-dioxolo[4,5-b]phenazin-6(7H)-yl)carbonyl]- (9CI)
ED Entered STN: 28 Jan 2005
LC STN Files: CHEMCATS

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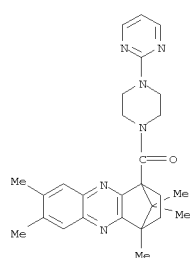
L33 ANSWER 9 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 821811-31-8 REGISTRY
 CN Methanone, (8,9-dihydro-9,12,12-trimethyl-6,9-methano-1,3-dioxolo[4,5-b]phenazin-6(7H)-yl)(4-phenyl-1-piperazinyl)- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Piperazine,
 1-[(8,9-dihydro-9,12,12-trimethyl-6,9-methano-1,3-dioxolo[4,5-b]phenazin-6(7H)-yl)carbonyl]-4-phenyl- (9CI)
 ED Entered STN: 28 Jan 2005
 LC STN Files: CHEMCATS

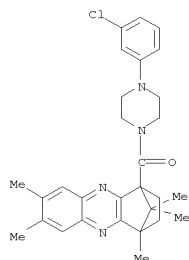
L33 ANSWER 10 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 821810-20-2 REGISTRY
 CN Methanone, [4-(2-pyrimidinyl)-1-piperazinyl](1,2,3,4-tetrahydro-4,7,8,11,11-pentamethyl-1,4-methanophenazin-1-yl)- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Piperazine, 1-[(3,4-dihydro-4,7,8,11,11-pentamethyl-1,4-methanophenazin-1(2H)-yl)carbonyl]-4-(2-pyrimidinyl)- (9CI)
 ED Entered STN: 28 Jan 2005
 LC STN Files: CHEMCATS

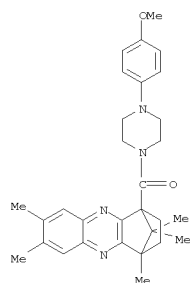
L33 ANSWER 11 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 821016-63-1 REGISTRY
 CN Methanone, [4-(3-chlorophenyl)-1-piperazinyl](1,2,3,4-tetrahydro-4,7,8,11,11-pentamethyl-1,4-methanophenazin-1-yl)- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Piperazine,
 1-(3-chlorophenyl)-4-[(3,4-dihydro-4,7,8,11,11-pentamethyl-1,4-methanophenazin-1(2H)-yl)carbonyl]- (9CI)
 ED Entered STN: 27 Jan 2005
 LC STN Files: CHEMCATS

L33 ANSWER 12 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN

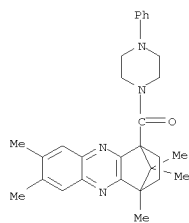


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 821016-61-9 REGISTRY
 CN Methanone, [4-(4-methoxyphenyl)-1-piperazinyl](1,2,3,4-tetrahydro-4,7,8,11,11-pentamethyl-1,4-methanophenazin-1-yl)- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Piperazine, 1-[(3,4-dihydro-4,7,8,11,11-pentamethyl-1,4-methanophenazin-1(2H)-yl)carbonyl]-4-(4-methoxyphenyl)- (9CI)
 ED Entered STN: 27 Jan 2005
 LC STN Files: CHEMCATS

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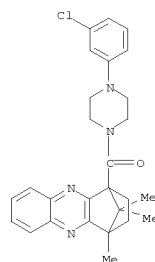
L33 ANSWER 13 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 821016-55-1 REGISTRY
 CN Methanone, (4-phenyl-1-piperazinyl) (1,2,3,4-tetrahydro-4,7,8,11,11-pentamethyl-1,4-methanophenazin-1-yl)- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Piperazine, 1-[(3,4-dihydro-4,7,8,11,11-pentamethyl-1,4-methanophenazin-1(2H)-yl)carbonyl]-4-phenyl- (9CI)
 ED Entered STN: 27 Jan 2005
 LC STN Files: CHEMCATS

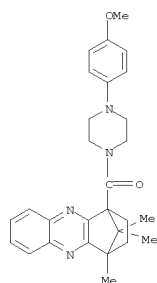
L33 ANSWER 14 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 622824-47-9 REGISTRY
 CN Methanone, [4-(3-chlorophenyl)-1-piperazinyl] (1,2,3,4-tetrahydro-4,11,11-trimethyl-1,4-methanophenazin-1-yl)- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Piperazine, 1-(3-chlorophenyl)-4-[(3,4-dihydro-4,11,11-trimethyl-1,4-methanophenazin-1(2H)-yl)carbonyl]- (9CI)
 ED Entered STN: 02 Dec 2003
 LC STN Files: CHEMCATS

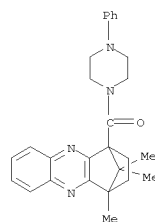
L33 ANSWER 15 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 622824-43-5 REGISTRY
 CN Methanone, [4-(4-methoxyphenyl)-1-piperazinyl] (1,2,3,4-tetrahydro-4,11,11-trimethyl-1,4-methanophenazin-1-yl)- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Piperazine, 1-[(3,4-dihydro-4,11,11-trimethyl-1,4-methanophenazin-1(2H)-yl)carbonyl]-4-(4-methoxyphenyl)- (9CI)
 ED Entered STN: 02 Dec 2003
 LC STN Files: CHEMCATS

L33 ANSWER 16 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN

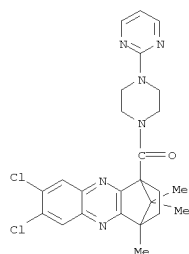


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 622824-31-1 REGISTRY
 CN Methanone, (4-phenyl-1-piperazinyl) (1,2,3,4-tetrahydro-4,11,11-trimethyl-1,4-methanophenazin-1-yl)- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Piperazine, 1-[(3,4-dihydro-4,11,11-trimethyl-1,4-methanophenazin-1(2H)-yl)carbonyl]-4-phenyl- (9CI)
 ED Entered STN: 02 Dec 2003
 LC STN Files: CHEMCATS

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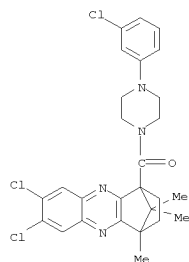
L33 ANSWER 17 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 622823-97-6 REGISTRY
CN Methanone, (7,8-dichloro-1,2,3,4-tetrahydro-4,11,11-trimethyl-1,4-methanophenazin-1-yl) [4-(2-pyrimidinyl)-1-piperazinyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[(7,8-dichloro-3,4-dihydro-4,11,11-trimethyl-1,4-methanophenazin-1(2H)-yl)carbonyl]-4-(2-pyrimidinyl)- (9CI)
ED Entered STN: 02 Dec 2003
LC STN Files: CHEMCATS

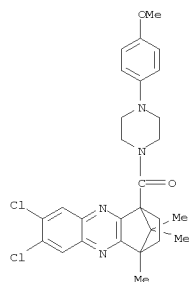
L33 ANSWER 18 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 622820-38-6 REGISTRY
CN Methanone, [4-(3-chlorophenyl)-1-piperazinyl] (7,8-dichloro-1,2,3,4-tetrahydro-4,11,11-trimethyl-1,4-methanophenazin-1-yl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-(3-chlorophenyl)-4-[(7,8-dichloro-3,4-dihydro-4,11,11-trimethyl-1,4-methanophenazin-1(2H)-yl)carbonyl]- (9CI)
ED Entered STN: 02 Dec 2003
LC STN Files: CHEMCATS

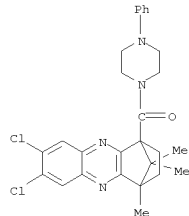
L33 ANSWER 19 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 622820-33-1 REGISTRY
CN Methanone, (7,8-dichloro-1,2,3,4-tetrahydro-4,11,11-trimethyl-1,4-methanophenazin-1-yl) [4-(4-methoxyphenyl)-1-piperazinyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[(7,8-dichloro-3,4-dihydro-4,11,11-trimethyl-1,4-methanophenazin-1(2H)-yl)carbonyl]-4-(4-methoxyphenyl)- (9CI)
ED Entered STN: 02 Dec 2003
LC STN Files: CHEMCATS

L33 ANSWER 20 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN

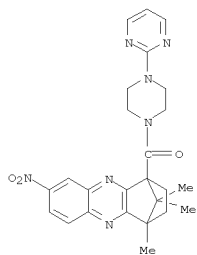


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 622820-18-2 REGISTRY
CN Methanone, (7,8-dichloro-1,2,3,4-tetrahydro-4,11,11-trimethyl-1,4-methanophenazin-1-yl) (4-phenyl-1-piperazinyl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[(7,8-dichloro-3,4-dihydro-4,11,11-trimethyl-1,4-methanophenazin-1(2H)-yl)carbonyl]-4-phenyl- (9CI)
ED Entered STN: 02 Dec 2003
LC STN Files: CHEMCATS

10590585.trn

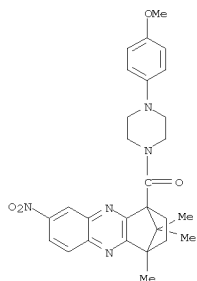
L33 ANSWER 21 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 622814-21-5 REGISTRY
CN Methanone, [4-(2-pyrimidinyl)-1-piperazinyl](1,2,3,4-tetrahydro-4,11,11-trimethyl-8-nitro-1,4-methanophenazin-1-yl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine,
1-[(3,4-dihydro-4,11,11-trimethyl-8-nitro-1,4-methanophenazin-1(2H)-yl)carbonyl]-4-(2-pyrimidinyl)- (9CI)
ED Entered STN: 02 Dec 2003
LC STN Files: CHEMCATS

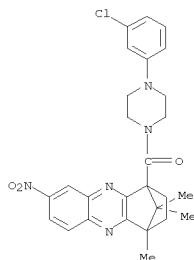
L33 ANSWER 23 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 622808-26-8 REGISTRY
CN Methanone,
[4-(4-methoxyphenyl)-1-piperazinyl](1,2,3,4-tetrahydro-4,11,11-trimethyl-8-nitro-1,4-methanophenazin-1-yl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine,
1-[(3,4-dihydro-4,11,11-trimethyl-8-nitro-1,4-methanophenazin-1(2H)-yl)carbonyl]-4-(4-methoxyphenyl)- (9CI)
ED Entered STN: 02 Dec 2003
LC STN Files: CHEMCATS

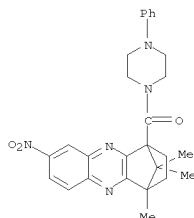
L33 ANSWER 22 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 622808-33-7 REGISTRY
CN Methanone, [4-(3-chlorophenyl)-1-piperazinyl](1,2,3,4-tetrahydro-4,11,11-trimethyl-8-nitro-1,4-methanophenazin-1-yl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-(3-chlorophenyl)-4-[(3,4-dihydro-4,11,11-trimethyl-8-nitro-1,4-methanophenazin-1(2H)-yl)carbonyl]- (9CI)
ED Entered STN: 02 Dec 2003
LC STN Files: CHEMCATS

L33 ANSWER 24 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN

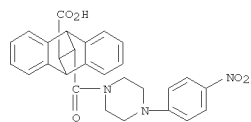


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 622808-05-3 REGISTRY
CN Methanone,
(4-phenyl-1-piperazinyl)(1,2,3,4-tetrahydro-4,11,11-trimethyl-8-nitro-1,4-methanophenazin-1-yl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine,
1-[(3,4-dihydro-4,11,11-trimethyl-8-nitro-1,4-methanophenazin-1(2H)-yl)carbonyl]-4-phenyl- (9CI)
ED Entered STN: 02 Dec 2003
LC STN Files: CHEMCATS

10590585.trn

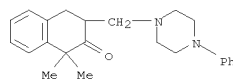
L33 ANSWER 25 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 332025-17-9 REGISTRY
CN 9,10-Ethanoanthracene-11-carboxylic acid,
9,10-dihydro-12-[[4-(4-nitrophenyl)-1-piperazinyl]carbonyl]- (CA INDEX
NAME)
ED Entered STN: 23 Apr 2001
LC STN Files: CHEMCATS

L33 ANSWER 26 OF 26 REGISTRY COPYRIGHT 2010 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

RN 7773-25-3 REGISTRY
CN 2(1H)-Naphthalenone, 3,4-dihydro-1,1-dimethyl-3-[(4-phenyl-1-
piperazinyl)methyl]- (CA INDEX NAME)
ED Entered STN: 16 Nov 1984
LC STN Files: BEILSTEIN*
(*File contains numerically searchable property data)

10590585.trn

=> file caplus

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REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2009

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L6	SCREEN 1840 AND 1992
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L8	QUE L7 AND L6
L9	0 S L8
L10	SCREEN 1992 AND 1840
L11	STRUCTURE UPLOADED
L12	QUE L11 AND L10
L13	1 S L12
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L15	2737850 S 46.156.1/RID
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L17	1 S PIPERAZINE/CN
L18	1597508 S 46.383.1/RID

10590585.trn

L19 90686 S L18 AND L15
L20 0 S SAM L12 SUB=L15
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L22 0 S FULL L12 SUB=L19
L23 372 S FULL L12 SUB=L18
L24 766 S L21 OR L23

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L31 1 S L28 AND BEILSTEIN/LC
L32 41 S L30 OR L31
L33 26 S L32 AND ED<=2005

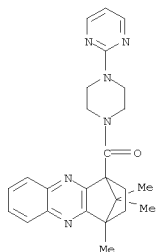
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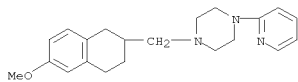
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L25 ANSWER 1 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2009:846112 Document No. 151:92849 Method using lifespan-altering compounds for altering the lifespan of eukaryotic organisms, and screening for such compounds. Goldfarb, David Scott (University of Rochester, USA). U.S. Pat. Appl. Publ. US 20090163545 A1 20090625, 57pp. (English). CODEN: USXXCO. APPLICATION: US 2008-XN341615 20081222. PRIORITY: US 2007-16362P 20071221; US 2008-23801P 20080125.
AB The invention discloses a method for altering the lifespan of a eukaryotic organism. The method comprises the steps of providing a lifespan-altering compound, and administering an effective amount of the compound to a eukaryotic organism, such that the lifespan of the organism is altered. In one embodiment, the compound is identified using the Dead assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]
IT 622365-06-4
RL: PAC (Pharmacological activity); BIOL (Biological study) (method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)
RN 622365-06-4 CAPLUS
CN Methanone, [4-(2-pyrimidinyl)-1-piperazinyl] (1,2,3,4-tetrahydro-4,11,11-trimethyl-1,4-methanophenazin-1-yl)- (CA INDEX NAME)

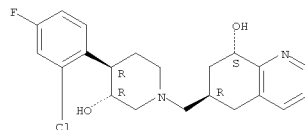


L25 ANSWER 3 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2008:1417101 Document No. 149:5482830 Novel 4-(4-Aryl)cyclohexyl-1-(2-pyridyl)piperazines as Δ^8 - Δ^7 Sterol Isomerase (Etopamil Binding Protein) Selective Ligands with Antiproliferative Activity. Berardi, Francesco; Abate, Carmen; Ferorelli, Savina; de Robertis, Anna F.; Leopoldo, Marcello; Colabufio, Nicola A.; Niso, Mauro; Perrone, Roberto (Dipartimento Farmacochimico, Università degli Studi di Bari, Bari, I-70125, Italy). Journal of Medicinal Chemistry, 51(23), 7523-7531 (English) 2008. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 149:548283. Publisher: American Chemical Society.
AB To find Δ^8 - Δ^7 sterol isomerase (EBP) selective ligands, various arylpiperazines previously studied and structurally related to some σ receptors ligands were preliminarily screened. Consequently, a novel series of 2- or 2,6-disubstituted (CH₃, CH₃O, Cl, F) cis- and trans-4-(4-aryl)cyclohexyl-1-(2-pyridyl)piperazines was developed. Radioreceptor binding assays evidenced cis-19, cis-30 and cis-33 as new ligands with nanomolar affinity toward EBP site and a good selectivity relative to EBP-related σ receptors. The most selective 2,6-dimethoxy derivative (cis-33) demonstrated the highest potency (EC₅₀ = 12.9 μ M) and efficacy (70%) in inhibiting proliferation of human prostate cancer PC-3 cell line. Among the reference compds., σ_2 agonist 36 (PB28) reached the maximum efficacy (100%), suggesting the contribution of the σ_2 receptor to the antiproliferative activity. This novel class of EBP inhibitors represents a valuable tool for investigating the last steps of cholesterol biosynthesis and related pathologies, as well as a starting point for developing new anticancer drugs.
IT 385811-17-6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (cyclohexyl pyridylpiperazines as Δ^8 - Δ^7 sterol isomerase ligands with antiproliferative activity)
RN 385811-17-6 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[(1,2,3,4-tetrahydro-6-methoxy-2-naphthalenyl)methyl]- (CA INDEX NAME)

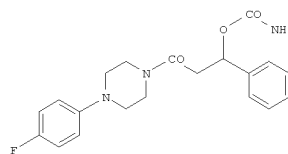
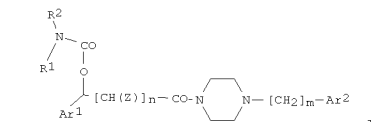


L25 ANSWER 2 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2009:753543 Document No. 151:1632230 Identification of an Orally Active Opioid Receptor-like 1 (ORL1) Receptor Antagonist
4-{3-[(2R)-2,3-Dihydroxypropyl]-2-oxo-2,3-dihydro-1H-benzimidazol-1-yl}-1-[(1S,3S,4R)-spiro[bicyclo[2.2.1]heptane-2,1'-cyclopropan]-3-ylmethyl]piperidine as Clinical Candidate. Satoh, Atsushi; Sagara, Takeshi; Sakoh, Hiroki; Hashimoto, Masaya; Nakashima, Hiroshi; Kato, Tetsuya; Goto, Yasuhiro; Mizutani, Sayaka; Azuma-Kanoh, Tomoko; Tani, Takeshi; Okuda, Shoki; Okamoto, Osamu; Ozaki, Satoshi; Iwasawa, Yoshikazu; Ohta, Hisashi; Kawamoto, Hiroshi (Tsukuba Research Institute, Banyu Pharmaceutical Co. Ltd., Okubo-3, Tsukuba 300-2611, Ibaraki, 300-2611, Japan). Journal of Medicinal Chemistry, 52(14), 4091-4094 (English) 2009. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 151:163223. Publisher: American Chemical Society.
AB Our efforts to optimize prototype opioid receptor-like 1 (ORL1) antagonist 1 led to the discovery of 4-{3-[(2R)-2,3-dihydroxypropyl]-2-oxo-2,3-dihydro-1H-benzimidazol-1-yl}-1-[(1S,3S,4R)-spiro[bicyclo[2.2.1]heptane-2,1'-cyclopropan]-3-ylmethyl]piperidine 10. 10 Showed potent ORL1 antagonistic activity, excellent selectivity over other opioid receptors, and in vivo efficacy after oral dosing. Currently clin. trials of 10 are underway.
IT 864830-99-9
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (orally active ORL1 antagonists preparation)
RN 864830-99-9 CAPLUS
CN 8-Quinololinol, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-piperidinyl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)- (CA INDEX NAME)

Absolute stereochemistry.

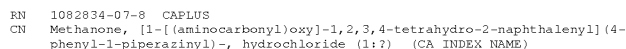


L25 ANSWER 4 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2008:1398511 Document No. 149:5765880 Novel carbamoyloxy arylalkanoil arylpiperazine compound, pharmaceutical compositions comprising the compound and method for treating pain, anxiety and depression by administering the compound. Kwak, Byong Sung; Moon, Hong Sik; Yi, Han-Ju; Kang, Young Soon; Im, Dae Joong; Chae, Eun Hee; Chae, Sang Mi; Lee, Ki Ho (SK Holdings Co., Ltd., S. Korea). PCT Int. Appl. WO 2008140198 A1 20081120, 62pp. DESIGNATED STATES: W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IS, IT, LU, MC, ML, MR, MT, NE, NL, NO, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2008-KR2470 20080430. PRIORITY: KR 2007-46708 20070514.
GI



AB There is provided a novel carbamoyloxy arylalkanoil arylpiperazine derivative compound having abundant racemic or enantiomeric characteristics, represented by the Formula I (wherein R1 and R2 are independently H, Cl-C6 alkyl, and phenethyl, or together form part of a ring; Ar1 is furanyl, thionyl, methylenedioxyphenyl, and Ph that may be substituted; Z is H or F, or together with Ar1 forms a bicyclic ring; Ar2 is Ph, methylenedioxyphenyl, etc.; n is 1 or 2; and m is 0-2), and pharmaceutically available salts or hydrates thereof. Also, there are provided a pharmaceutical composition for treating pain, anxiety or depression including an effective amount of the compound, and a method for treating pain, anxiety or depression in mammals by administering an effective amount of the

L25	ANSWER 4 OF 96 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued) compd. to the MAPPLS IN NEED of treatment thereof. Synthetic procedures for prep. I are exemplified. Example compd. II was prep. via a multi-step synthesis starting with the reaction between Et benzoylacetate and 4-fluorophenylpiperazine. In an acetic acid-induced writing test in mice, II (10 mg/kg, p.o.) inhibited pain by 73.5 %.
IT	1082831-66-OP, Carbamate acid 2-((4-phenylpiperazin-1-yl) carbonyl)-1,2,3,4-tetrahydronaphthalen-1-yl ester 1082834-07-8P 1082834-09-OP RL: PAC (Pharmacological activity); SFN (Synthetic preparation); THU (Therapeutic use); BLOL (Biological study); PREP (Preparation); USES (Uses) (drug candidate; preparation of carbamoyloxy arylalkanoyl aryl piperazine compds. for treating pain, anxiety and depression)
RN	1082831-66-0 CAPLUS
CN	Methanone, [1-(aminocarbonyl)-1',2',3',4'-tetrahydro-2-naphthalenyl] (4- phenyl-piperazinyl)- (CA INDEX NAME)



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RN      1082834-09-0    CAPLUS
CN      Methanone, [1-[(aminocarbonyl)oxy]-1,2,3,4-tetrahydro-2-naphthalenyl] (4-
        phenyl-1-piperazinyl)-, methanesulfonate (1:?) (CA INDEX NAME)

CM      1

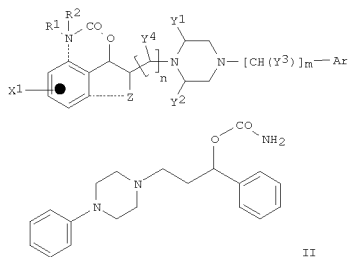
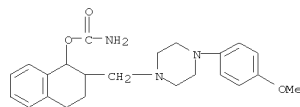
CRN     1082831-66-0

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CM	2
CRN	75-75-2
CMF	C H4 O3 S



L25 ANSWER 5 OF 96 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)
reaction between acetophenone and phenylpiperazine. In an acetic
acid-induced writhing test in mice, II had an ED50 of 6.31 po in
suppressing pain.
IT 1083076-22-5P, Carbamic acid
2-[[4-(4-methoxyphenyl)piperazin-1-yl]methyl]-1,2,3,4-tetrahydronaphthalen-
1-yl ester
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(drug candidate; preparation of carbamoyloxy arylalkane arylpiperazine
comps. for treating pain, anxiety and depression)
FN 1083076-22-5 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-2-[[4-(4-methoxyphenyl)-1-
piperazinyl]methyl]-, 1-carbamate (CAS INDEX NAME)



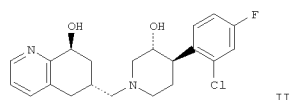
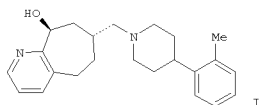
AB There is provided a novel carbanoyloxy arylalkan arylpiperazine derivative compound having abundant racemic or enantiomeric characteristics, represented by the formula I (wherein --- may selectively form a cyclic ring; R1 and R2 are H or together with X1 form a bicyclic ring; the ring labeled X1 may be (un)substituted Ph or a bicyclic ring; Z is H or F or together with X1 forms a bicyclic ring; Ar is (un)substituted Ph, pyridine, pyrimidine, etc.; Y1 and Y2 are independently H or Me; Y3 is H, Ph, or CO; Y4 is H or Me; n is 1 or 2; and m is 0 or 1), and pharmaceutically available salts or hydrates thereof. Also, there are provided a pharmaceutical composition for treating pain (i.e., acute or chronic pain, neuropathic pain, inflammatory pain, diabetic pain, postherpetic neuralgia, etc.), anxiety or depression including an effective amount of the compound, and a method for treating pain, anxiety or depression in mammals by administering an effective amount of the compound to the mammals in need of treatment thereof. Synthetic procedures for preparing I are exemplified. Example compound II was prepared in a multistep synthesis from an initial

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L25 ANSWER 6 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2008:685859 Document No. 149:1761540 A Novel Class of
Cycloalkano[b]pyridines as Potent and Orally Active Opioid Receptor-like

1 Antagonists with Minimal Binding Affinity to the hERG K⁺ Channel.
Yoshizumi, Takashi; Takahashi, Hirobumi; Miyazoe, Hiroshi; Sugimoto,
Yuichi; Tsujita, Tomohiro; Kato, Tetsuya; Ito, Hirokatsu; Kawamoto,
Hiroshi; Hirayama, Miko; Ichikawa, Daisuke; Azuma-Kanoh, Tomoko; Ozaki,
Satoshi; Shibata, Yoshihiro; Tanl, Takeshi; Chiba, Masato; Ishii,
Yasuyuki; Okuda, Shoki; Tadano, Kiyoshi; Fukuroda, Takahiro; Okamoto,
Osamu; Ohta, Hisashi (Tsukuba Research Institute, Banyu Pharmaceutical
Co., Ltd, Okubo-3, Tsukuba, Ibaraki, 300-2611, Japan). Journal of
Medicinal Chemistry, 51(13), 4021-4029 (English) 2008. CODEN: JMCMAR.
ISSN: 0022-2623. OTHER SOURCES: CASREACT 149:176154. Publisher:
American
Chemical Society.

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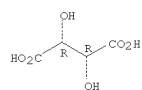
AB A series of compds. based on
7-[[4-(2-methylphenyl)piperidin-1-yl]methyl]-
6,7,8,9-tetrahydro-5H-cyclohepta[b]pyridine-9-ol ((-)-I), a potent and
selective opioid receptor-like 1 (ORL1) antagonist, was prepared and
evaluated using structure-activity relationship studies with the aim of
removing its affinity to human ether-a-go-go related gene (hERG) K⁺
channel. From these studies, II was identified as an optimized structure
with respect to ORL1 antagonist activity, and affinity to the hERG
K⁺channel. Furthermore, II showed good in vivo antagonism with a wide
therapeutic index in regards to adverse cardiovascular effects.

IT 864828-68-2P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP
(Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL
(Biological study); PREP (Preparation); USES (Uses)
(crystal structure; synthesis and biol. evaluation of
arylpyridinylmethyl-substituted cycloalkano[b]pyridines as orally
active opioid receptor-like 1 antagonists with minimal binding
affinity

L25 ANSWER 6 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.



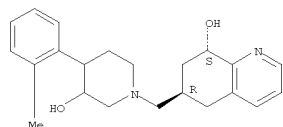
IT 1039359-51-7P 1039359-53-9P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic
preparation); BIOL (Biological study); PREP (Preparation)
(lipophilicity; synthesis and biol. evaluation of
arylpyridinylmethyl-substituted cycloalkano[b]pyridines as orally
active opioid receptor-like 1 antagonists with minimal binding
affinity

to the hERG K⁺ channel)
RN 1039359-51-7 CAPLUS
CN 8-Quinololinol, 5,6,7,8-tetrahydro-6-[[3-hydroxy-4-(2-methylphenyl)-1-
piperidinyl]methyl]-, (6R,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1)
(CA INDEX NAME)

CM 1

CRN 1039359-50-6
CMF C22 H28 N2 O2

Absolute stereochemistry.



CM 2

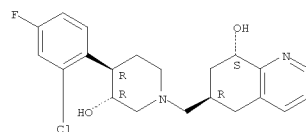
CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.

L25 ANSWER 6 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
to the hERG K⁺ channel)

RN 864828-68-2 CAPLUS
CN 8-Quinololinol, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-
piperidinyl]methyl]-5,6,7,8-tetrahydro-, hydrochloride (1:1), (6R,8S)-
(CA INDEX NAME)

Absolute stereochemistry.



● HCl

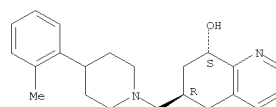
IT 1039359-49-3P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic
preparation); BIOL (Biological study); PREP (Preparation)
(lipophilicity and acidity; synthesis and biol. evaluation of
arylpyridinylmethyl-substituted cycloalkano[b]pyridines as orally
active opioid receptor-like 1 antagonists with minimal binding
affinity
to the hERG K⁺ channel)

RN 1039359-49-3 CAPLUS
CN 8-Quinololinol, 5,6,7,8-tetrahydro-6-[[4-(2-methylphenyl)-1-
piperidinyl]methyl]-, (6R,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1)
(CA INDEX NAME)

CM 1

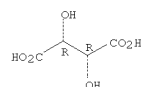
CRN 1039359-48-2
CMF C22 H28 N2 O

Absolute stereochemistry. Rotation (-).



CM 2

L25 ANSWER 6 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

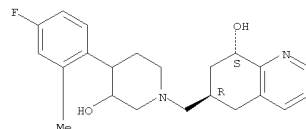


RN 1039359-53-9 CAPLUS
CN 8-Quinololinol, 6-[[4-(4-fluoro-2-methylphenyl)-3-hydroxy-1-
piperidinyl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)-,
(2R,3R)-2,3-dihydroxybutanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 1039359-52-8
CMF C22 H27 F N2 O2

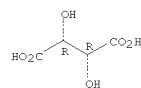
Absolute stereochemistry.



CM 2

CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.



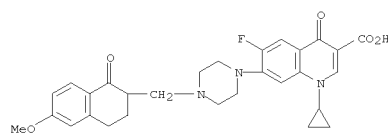
10590585.trn

L25 ANSWER 7 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2008;670939 Document No. 149;100450 Synthesis of quinoline derivatives with
 antibacterial activity. Srivastava, Brijesh K.; Jain, Mukul R.; Patel,
 Pankaj R. (Cadila Healthcare Limited, India). Eur. Pat. Appl. EP 1927589
 A1 20080604, 19pp. DESIGNATED STATES: R: AT, BE, BG, CH, CY, CZ, DE,
 DK,
 EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, PL,
 PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, RS. (English). CODEN: EPXXDW.
 APPLICATION: EP 2007-254643 20071130. PRIORITY: IN 2006-MU1967 20061130.
 GI

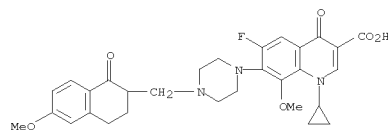
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention relates to a process for preparing quinoline
 compds. I
 [R1 = H, (C1-C12)alkyl, (C3-C12)cycloalkyl; R2, R3 = H, OH, halo, alkoxy,
 NO2, cyano; R8, R9, R10, R11 = H, alkyl; R4, R5, R6, R7 = H, halo,
 haloalkyl, OH, alkoxy, thio NO2, cyano, amino, (C1-C12)alkyl,
 (C1-C12)alkoxy derivative of sulfenyl or sulfonyl group, sulfonic acid
 and
 derivs.; Z = O, S, NR, R = H, OH, (C1-C3)alkyl; X = absent or CH2, O, S,
 SO, SO2; Y = (CH2)n, n = 0-3], their tautomeric forms, their
 pharmaceutically acceptable salts and pharmaceutical compns. containing
 them.
 For example, reacting 6-methoxy- α -tetralone with quinolinecarboxylic
 acid II gave piperazinyl quinoline III in 75% yield. Compound III and
 analog IV were tested for antibacterial activity; their pharmacokinetic
 profile was also explored.
 IT 1029844-02-7P, 1-Cyclopropyl-6-fluoro-7-[4-[(6-methoxy-1-oxo-
 1,2,3,4-tetrahydronaphthalen-2-yl)methyl]piperazin-1-yl]-4-oxo-1,4-
 dihydroquinoline-3-carboxylic acid 1029844-06-1P,
 RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); RCT
 (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL
 (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES
 (Uses)
 (preparation of (oxoquinolinyl)piperazine derivs. and their
 antibacterial
 activity)
 RN 1029844-02-7 CAPLUS
 CN 3-Quinolinecarboxylic acid,
 1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-[4-
 [(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-piperazinyl]-
 (CA INDEX NAME)

L25 ANSWER 7 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

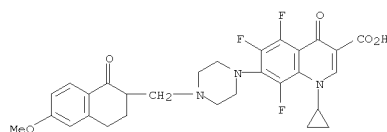


IT 1029844-04-9P, 1-Cyclopropyl-6-fluoro-8-methoxy-7-[4-[(6-methoxy-
 1-oxo-1,2,3,4-tetrahydronaphthalen-2-yl)methyl]piperazin-1-yl]-4-oxo-1,4-
 dihydroquinoline-3-carboxylic acid 1029844-05-0P,
 1-Cyclopropyl-5,6,8-trifluoro-7-[4-[(6-methoxy-1-oxo-1,2,3,4-
 tetrahydronaphthalen-2-yl)methyl]piperazin-1-yl]-4-oxo-1,4-
 dihydroquinoline-3-carboxylic acid 1029844-06-1P,
 1-Cyclopropyl-6-fluoro-8-methoxy-7-[4-[(6-methoxy-1-oxo-1,2,3,4-
 tetrahydronaphthalen-2-yl)methyl]-3-methylpiperazin-1-yl]-4-oxo-1,4-
 dihydroquinoline-3-carboxylic acid 1029844-07-2P,
 1-Ethyl-6-fluoro-7-[4-[(6-methoxy-1-oxo-1,2,3,4-tetrahydronaphthalen-2-
 yl)methyl]piperazin-1-yl]-4-oxo-1,4-dihydroquinoline-3-carboxylic acid
 1029844-18-5P, 1-Cyclopropyl-6-fluoro-7-[4-[(1-hydroxyimino-6-
 methoxy-1,2,3,4-tetrahydronaphthalen-2-yl)methyl]piperazin-1-yl]-4-oxo-1,4-
 dihydroquinoline-3-carboxylic acid
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (preparation of (oxoquinolinyl)piperazine derivs. and their
 antibacterial
 activity)
 RN 1029844-04-9 CAPLUS
 CN 3-Quinolinecarboxylic acid,
 1-cyclopropyl-6-fluoro-1,4-dihydro-8-methoxy-4-
 oxo-7-[4-[(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-
 piperazinyl]- (CA INDEX NAME)

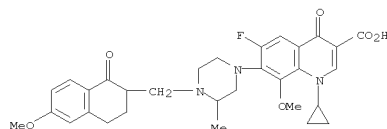


RN 1029844-05-0 CAPLUS
 CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-5,6,8-trifluoro-1,4-dihydro-4-
 oxo-7-[4-[(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-
 piperazinyl]- (CA INDEX NAME)

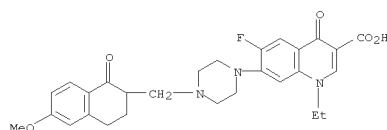
L25 ANSWER 7 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 1029844-06-1 CAPLUS
 CN 3-Quinolinecarboxylic acid,
 1-cyclopropyl-6-fluoro-1,4-dihydro-8-methoxy-7-
 [3-methyl-4-[(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-
 piperazinyl]-4-oxo- (CA INDEX NAME)

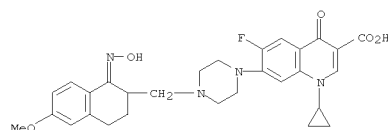


RN 1029844-07-2 CAPLUS
 CN 3-Quinolinecarboxylic acid, 1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-[4-
 [(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-piperazinyl]-
 (CA INDEX NAME)



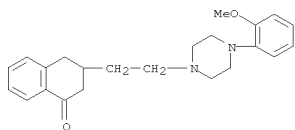
RN 1029844-18-5 CAPLUS
 CN 3-Quinolinecarboxylic acid,
 1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-[4-
 [(1,2,3,4-tetrahydro-1-(hydroxyimino)-6-methoxy-2-naphthalenyl)methyl]-1-
 piperazinyl]- (CA INDEX NAME)

L25 ANSWER 7 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



10590585.trn

L25 ANSWER 8 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2008:366390 Document No. 149:95648 Quantitative structure - activity relationship studies on membrane receptors inhibition by antipsychotic drugs. Application to schizophrenia treatment. Avram, Speranta; Berner, Heinz; Milac, Adina L.; Wolschann, Peter (Department of Physiology and Biophysics, Faculty of Biology, University of Bucharest, Bucharest, Rom.). Monatshefte fuer Chemie, 139(4), 407-426 (English) 2008. CODEN: MOCMB7. ISSN: 0026-9247. Publisher: Springer Wien.
 AB There are presented 6 new QSAR models, which are correlating antipsychotic activity (pK_i values at dopamine D1-D4 and serotonin (5-HT_{2C}, 5-HT_{2A}) receptors) with physicochem. parameters. A large data set of typical and atypical antipsychotics already approved for clin. treatment including as well representatives with new chemical structures which are exhibiting antipsychotic activity (tetrahydrofuran-, benzamide-, 3-aminoethyl-1-tetralones-, piperazine-, benzothiazepine- and pyrrolobenzazepine-derivs.) were incorporated within this study. The appropriate 2D and internal-3D mol. descriptors could be generated by the computational software MOE (Mol. Operating Environment). Significant q₂ (0.63-0.76) and r₂ (0.70-0.78) correlation coeffs. were obtained, indicating that the established equations can be used within a wide range of binding const. (pK_i = 5 to 9.76). By use of these linear models an assembly of new aripiprazole structures could be established. Some of them are showing significantly improved antipsychotic activity in comparison with the parent compound.
 IT 861804-06-0 861804-07-1 861804-08-2
 861804-09-3
 RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (QSAR studies on membrane receptors inhibition by antipsychotic drugs)
 RN 861804-06-0 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[2-[4-(2-methoxyphenyl)-1-piperazinyl]ethyl]- (CA INDEX NAME)



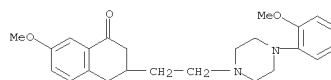
RN 861804-07-1 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-7-methoxy-3-[2-[4-(2-methoxyphenyl)-1-piperazinyl]ethyl]- (CA INDEX NAME)

L25 ANSWER 9 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2007:1028078 Document No. 147:5419990 Natural Products in Parallel Chemistry
 - Novel 5-Lipoxygenase Inhibitors from BIOS-Based Libraries Starting from α -santonin. Schwarz, Oliver; Jakupovic, Sven; Ambrosi, Horst-Dieter; Haustedt, Lars Ole; Mang, Christian; Mueller-Kuhrt, Lutz (Analyticon Discovery GmbH, Potsdam, 14473, Germany). Journal of Combinatorial Chemistry, 9(6), 1104-1113 (English) 2007. CODEN: JCCHFF. ISSN: 1520-4766. OTHER SOURCES: CASREACT 147:541999. Publisher: American Chemical Society.
 GI

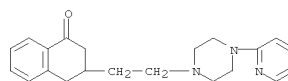
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Recently, we developed a concept known as biol.-oriented synthesis (BIOS), which targets the design and synthesis of small- to medium-sized compound libraries on the basis of genuine natural product templates to provide screening compds. with high biol. relevance. We herein describe the parallel solution phase synthesis of two BIOS-based libraries starting from α -santonin (I). Modification of the sesquiterpene lactone I by introduction of a thiazole moiety followed by a Lewis-acid-mediated lactone opening yielded a first library of natural product analogs, e.g. II. An acid-mediated dienone-phenol rearrangement of I and a subsequent etherification/amidation sequence led to a second natural product-based library, e.g. III. After application of a fingerprint-based virtual screening on these compds., the biol. screening of 23 selected library members against 5-lipoxygenase resulted in the discovery of four potent novel inhibitors of this enzyme.
 IT 956601-08-4P 956601-18-6P 956601-45-9P
 956601-46-0P
 RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)
 (BIOS-based library synthesis from α -santonin by introducing a thiazole moiety and lactone opening or rearrangement/etherification/amidation and their 5-lipoxygenase inhibitory activity)
 RN 956601-08-4 CAPLUS
 CN 1-Propanone, 1-[4-(4-fluorophenyl)-1-piperazinyl]-2-[(2R)-1,2,3,4-tetrahydro-7-methoxy-5,8-dimethyl-2-naphthalenyl]-, (2S)- (CA INDEX NAME)
 Absolute stereochemistry.

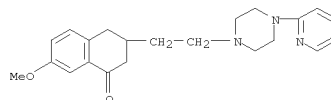
L25 ANSWER 8 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



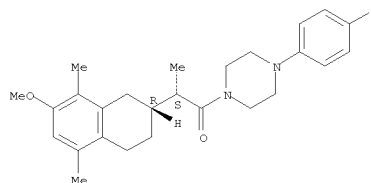
RN 861804-08-2 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[2-[4-(2-pyridinyl)-1-piperazinyl]ethyl]- (CA INDEX NAME)



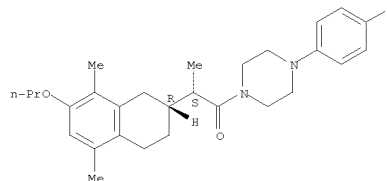
RN 861804-09-3 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-7-methoxy-3-[2-[4-(2-pyridinyl)-1-piperazinyl]ethyl]- (CA INDEX NAME)



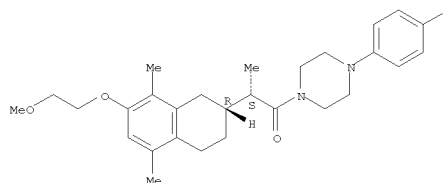
L25 ANSWER 9 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 956601-18-6 CAPLUS
 CN 1-Propanone, 1-[4-(4-fluorophenyl)-1-piperazinyl]-2-[(2R)-1,2,3,4-tetrahydro-5,8-dimethyl-7-propoxy-2-naphthalenyl]-, (2S)- (CA INDEX NAME)
 Absolute stereochemistry.



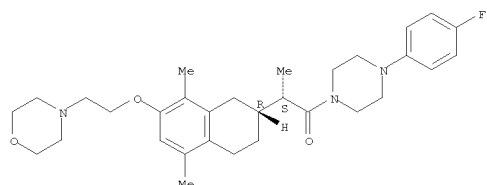
RN 956601-45-9 CAPLUS
 CN 1-Propanone, 1-[4-(4-fluorophenyl)-1-piperazinyl]-2-[(2R)-1,2,3,4-tetrahydro-7-(2-methoxyethoxy)-5,8-dimethyl-2-naphthalenyl]-, (2S)- (CA INDEX NAME)
 Absolute stereochemistry.



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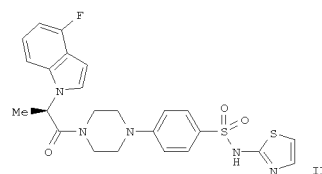
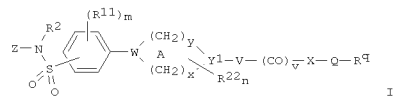
L25 ANSWER 9 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 RN 956601-46-0 CAPLUS
 CN 1-Propanone, 1-[4-(4-fluorophenyl)-1-piperazinyl]-2-[(2R)-1,2,3,4-tetrahydro-5,8-dimethyl-7-[2-(4-morpholinyl)ethoxy]-2-naphthalenyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



L25 ANSWER 10 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2007:730896 Document No. 147:1434680 Heterocyclic derivatives as modulators of ion channels and their preparation, pharmaceutical compositions and use in the treatment of diseases. Wilson, Dean; Fanning, Lev T.D.; Sheth, Urvil; Martinborough, Esther; Termin, Andreas; Neubert, Timothy; Zimmermann, Nicole; Knoll, Tara; Whitney, Tara; Kawatkar, Aarti; Lehsten, Danielle; Stamos, Dean; Zhou, Jinglan; Arumugam, Vijayalaksmi; Gutierrez, Corey (Vertex Pharmaceuticals Incorporated, USA). PCT Int. Appl. WO 2007/075895 A2 20070705, 369 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IS, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXDZ. APPLICATION: WO 2006-US48802 20061221. PRIORITY: US 2005-752926P 20051221; US 2006-791181P 20060411; US 2006-799797P 20060512; US 2006-839444P 20060823.

GI



AB The invention relates to heterocyclic derivs. of formula I useful as inhibitors of ion channels. Compound of formula I wherein Z is (un)substituted 5- to 7-membered (un)saturated heterocycle; W and Y1 are independently CH and H, provided that at least one of W and Y1 is N; x and y are independently 0 - 3, provided that x + y is 2, 3 and 4; m and n are

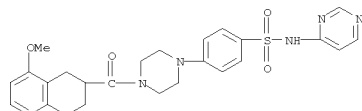
L25 ANSWER 10 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 independently 0 - 4; v is 0 and 1; Q is a bond, (un)branched (un)functionalized C1-6 alkylidene; Rq is (un)substituted C1-6 aliph., (un)substituted 3 to 8-membered (un)satd. mono(hetero)cycle, and (un)substituted 8- to 15-membered (un)satd. (bi/tri/spiro)(hetero)cycle; R11 is R2, halo, CN, NO2, CF3, OCF3, OH, etc.; R22 is R2, =O, =NHNH2 and derivs., =N-OH and derivs., OH and derivs., O-acyl, OCO2H and derivs., etc.; R2 is H, (un)substituted C1-6 aliph.; ring A may be optionally

fused with (un)substituted phenyl; and their pharmaceutically acceptable salts thereof, are claimed. The invention also provides pharmaceutically acceptable compns. comprising the compds. of the invention and methods of using the compns. in the treatment of various disorders. Compd. II was prepd. by acylation of 4-(piperazin-1-yl)-N-(thiazol-2-yl)benzenesulfonamide with (2R)-2-(fluoroindol-1-yl)propionic acid. All the invention compds. were evaluated for their sodium channel inhibitory activity.

IT 943651-27-2P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of heterocyclic derivs. as inhibitors of ion channels useful in treatment of various disorders)

RN 943651-27-2 CAPLUS
 CN Benzenesulfonamide, N-4-pyrimidinyl-4-[4-[(1,2,3,4-tetrahydro-8-methoxy-2-naphthalenyl)carbonyl]-1-piperazinyl]- (CA INDEX NAME)



L25 ANSWER 11 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2007:655407 Document No. 147:2498640 Multistucture 3D-QSAR Studies on a Series of Conformationally Constrained Butyrophenones Docked into a New Homology Model of the 5-HT2A Receptor. Dezi, Cristina; Brea, Jose; Alvarado, Mario; Ravina, Enrique; Masquer, Christian F.; Loza, Maria Isabel; Sanz, Ferran; Pastor, Manuel (Research Unit on Biomedical Informatics (GRIB), IMIM, Universitat Pompeu Fabra, Barcelona, E-08003, Spain). Journal of Medicinal Chemistry, 50(14), 3242-3255 (English) 2007.

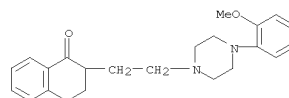
CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 147:249864. Publisher: American Chemical Society.
 AB The present study is part of a long-term research project aiming to gain insight into the mechanism of action of atypical antipsychotics. Here we describe a 3D-QSAR study carried out on a series of butyrophenones with affinity for the serotonin-2A receptor, aligned by docking into the binding site of a receptor model. The series studied has two peculiarities: (i) all the compds. have a chiral center and can be represented by two enantiomeric structures, and (ii) many of the structures can bind the receptor in two alternative orientations, posing the problem of how to select a single representative structure for every compound. We have used an original solution consisting of the simultaneous use

of multiple structures, representing different configurations, binding conformations, and positions. The final model showed good statistical quality (n = 426, r2 = 0.84, q2LOO = 0.81) and its interpretation provided useful information, not obtainable from the simple inspection of the ligand-receptor complexes.

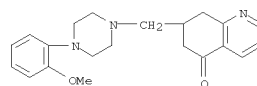
IT 149247-12-1 325489-07-4 676139-12-1
 676139-13-2 861804-06-0 861804-07-1
 861804-09-3

RL: PAC (Pharmacological activity); BIOL (Biological study) (multistucture QSAR studies on conformationally constrained butyrophenones docked into homol. model of 5-HT2A receptor)

RN 149247-12-1 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[2-[4-(2-methoxyphenyl)-1-piperazinyl]ethyl]- (CA INDEX NAME)



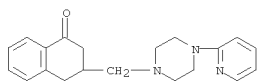
RN 325489-07-4 CAPLUS
 CN 5(6H)-Quinolone, 7,8-dihydro-7-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



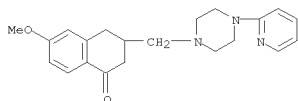
10590585.trn

L25 ANSWER 11 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

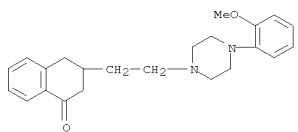
RN 676139-12-1 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[[4-(2-pyridinyl)-1-piperazinyl]methyl]-
(CA INDEX NAME)



RN 676139-13-2 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-3-[[4-(2-pyridinyl)-1-piperazinyl]methyl]-
(CA INDEX NAME)



RN 861804-06-0 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[2-[4-(2-methoxyphenyl)-1-piperazinyl]ethyl]-
(CA INDEX NAME)



RN 861804-07-1 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-7-methoxy-3-[2-[4-(2-methoxyphenyl)-1-piperazinyl]ethyl]-
(CA INDEX NAME)

L25 ANSWER 12 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN

2007:61266 Document No. 146:1630230 Preparation of oxyacids and oxyacid esters as serotonin receptor modulators.. Klaveness, Jo; Brudeli, Bjame; Levy, Finn Olav (Bio-Medizinsk Innovasjon AS, Norway; Cockbain, Julian). PCT Int. Appl. WO 2007007072 A1 20070118, 107pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IS, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2006-02542 20060707. PRIORITY: US 2005-696780P 20050707.

AB Oxyacid and oxyacid ester serotonin modulators were prepared. Thus, indole-3-carboxylic acid in CH₂Cl₂ was stirred 2 h with (COCl)₂ and cat. DMF; the residue in THF/CH₂Cl₂ was added dropwise to 4-(4-hydroxymethylpiperidin-1-yl)butyric acid 2,2,2-trichloroethyl ester (preparation given) and Et₃N in CH₂Cl₂ followed by stirring overnight to

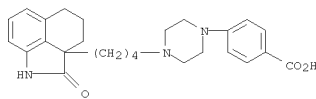
give 25.6% 1H-indole-3-carboxylic acid 1-[3-(2,2,2-trichloroethylethoxycarbonyl)propyl]piperidine-4-ylmethyl ester. The latter showed 5-HT₄ antagonist activity with pK_B = 9.13, vs. piboserod which showed pK_B = 9.26.

IT 1057307-69-3

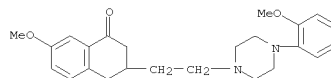
RL: PRPH (Prophetic)
(Preparation of oxyacids and oxyacid esters as serotonin receptor modulators.)

RN 1057307-69-3 CAPLUS

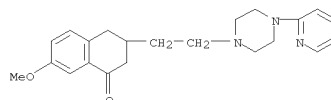
CN Benzoic acid, 4-[4-[(1,2,4,5-tetrahydro-2-oxobenz[cd]indol-2a(3H)-yl)butyl]-1-piperazinyl]-
(CA INDEX NAME)



L25 ANSWER 11 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



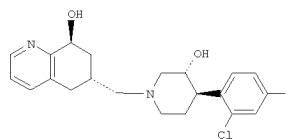
RN 861804-09-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-7-methoxy-3-[2-[4-(2-pyridinyl)-1-piperazinyl]ethyl]-
(CA INDEX NAME)



L25 ANSWER 13 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN

2006:941104 Document No. 145:335937 Preparation of A-form crystals of tetrahydroquinoline derivative and their medical compositions and pharmaceuticals. Sugimoto, Yuichi; Miyazoe, Hiroshi; Tsujita, Tomohiro (Banyu Pharmaceutical Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2006241096 A 20060914, 16pp. (Japanese). CODEN: JKXAF. APPLICATION: JP 2005-60632 20050304.

GI



I

AB A-form crystals of I.HCl are useful for prophylactic or therapeutic treatment of nociceptin receptor-associated diseases, e.g., pain, obesity,

impaired learning, dementia, schizophrenia, depression, etc. Thus, trimethylsilylated I was deprotected, converted into HCl salt in MeOH,

the solvent evaporated, dissolved in EtOH and treated with n-heptane to give A-form crystals of I.HCl, which inhibited the binding of [125I]-Tyr14-nociceptin to its receptor with IC₅₀ value of 9.00 nM. The

X

ray powder diffraction pattern of the crystals is also described.

IT 864828-68-2P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of A-form crystals of tetrahydroquinoline derivative as nociceptin receptor antagonist)

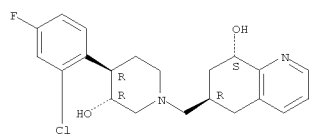
RN 864828-68-2 CAPLUS

CN 8-Quinololinol, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-piperidinyl]methyl]-5,6,7,8-tetrahydro-, hydrochloride (1:1), (6R,8S)-
(CA INDEX NAME)

Absolute stereochemistry.

10590585.trn

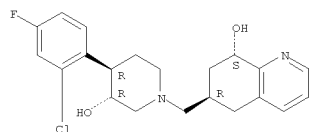
L25 ANSWER 13 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● HCl

IT 864830-99-9P 909781-64-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of A-form crystals of tetrahydroquinoline derivative as
 nociceptin
 receptor antagonist)
 RN 864830-99-9 CAPLUS
 CN 8-Quinolinol, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-
 piperidinyl)methyl]-5,6,7,8-tetrahydro-, (6R,8S)- (CA INDEX NAME)

Absolute stereochemistry.



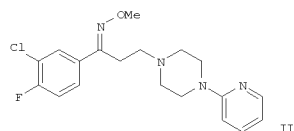
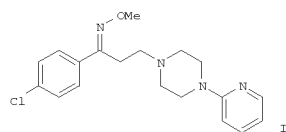
RN 909781-64-2 CAPLUS
 CN 3-Piperidinol,
 4-(2-chloro-4-fluorophenyl)-1-[[[(6R,8S)-5,6,7,8-tetrahydro-
 8-[(triethylsilyl)oxy]-6-quinolinyl)methyl]-, (3R,4R)- (CA INDEX NAME)

Absolute stereochemistry.

L25 ANSWER 14 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2006:729384 Document No. 145:3276470

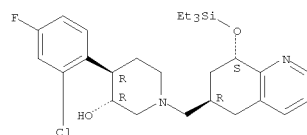
1-Aryl-3-(4-pyridine-2-ylpiperazin-1-yl)propan-1-one Oximes as Potent
 Dopamine D4 Receptor Agonists for the Treatment of Erectile Dysfunction.
 Kolasa, Teodorzyj; Matulenko, Mark A.; Hakeem, Ahmed A.; Patel, Meena V.;
 Mortell, Kathleen; Bhatia, Pramila; Henry, Rodger; Nakane, Masaki; Hsieh,
 Gin C.; Terranova, Marc A.; Uchic, Marie E.; Miller, Loan N.; Chang,
 Renje; Donnelly-Roberts, Diana L.; Namovic, Marian T.; Hollingsworth,
 Peter R.; Martino, Brenda; El Kouhen, Odile; Marsh, Kennan C.; Wetter,
 Jill M.; Moreland, Robert B.; Brioni, Jorge D.; Stewart, Andrew O.
 (Neuroscience Research, Abbott Laboratories, Abbott Park, IL, 60064-6101,
 USA). Journal of Medicinal Chemistry, 49(17), 5093-5109 (English) 2006.
 CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 145:327647.
 Publisher: American Chemical Society.

GI



AB A new series of dopamine D4 receptor agonists,
 1-aryl-3-(4-pyridinepiperazin-1-yl)propanone oximes, was designed through
 the modification of known dopamine D4 receptor agonist PD 168077.
 Replacement of the amide group with a methylene-oxime moiety produced
 comds. with improved stability and efficacy. Structure-activity
 relationships (SAR) of the aromatic ring linked to the N-4-piperazine
 ring confirmed the superiority of 2-pyridine as a core for D4 agonist
 activity.
 A two-methylene linker between the oxime group and the N-1-piperazine
 ring displayed the best profile. New dopamine D4 receptor agonists,
 exemplified by (E)-1-(4-chlorophenyl)-3-(4-pyridin-2-ylpiperazin-1-
 yl)propan-1-one O-methylloxime (I) (59a) and
 (E)-1-(3-chloro-4-fluorophenyl)-3-(4-pyridin-2-ylpiperazin-1-yl)propan-1-
 one O-methylloxime (II) (64a), exhibited favorable pharmacokinetic
 profiles
 and showed oral bioavailability in rat and dog. Subsequent evaluation of
 59a in the rat penile erection model revealed in vivo activity,
 comparable

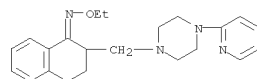
L25 ANSWER 13 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



L25 ANSWER 14 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

a novel structural linker for 4-arylpiperazine-based D4 agonists,
 possessing leadlike quality and with potential to develop a new class of potent and
 selective dopamine D4 receptor agonists.

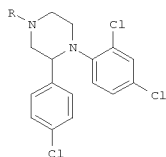
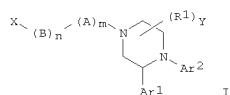
IT 909414-28-4P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (1-Aryl-3-(4-pyridine-2-ylpiperazin-1-yl)propan-1-one Oximes as Potent
 Dopamine D4 Receptor Agonists for the Treatment of Erectile
 Dysfunction)
 RN 909414-28-4 CAPLUS
 CN 1(2H)-Naphthalenone,
 3,4-dihydro-2-[[[4-(2-pyridinyl)-1-piperazinyl)methyl]-
 , O-ethyloxime (CA INDEX NAME)



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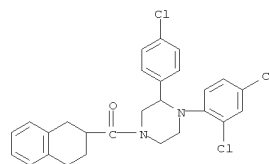
L25 ANSWER 15 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2006:542524 Document No. 145:460880 Substituted piperazines as CB1
 antagonists and their preparation, pharmaceutical compositions, and their
 use for treatment of metabolic disorders. Gilbert, Eric J.; Miller,
 Michael W.; Scott, Jack D.; Stamford, Andrew W.; Greenlee, William J.;
 Weinstein, Jay (Schering Corp., USA). PCT Int. Appl. WO 2006060461 A1
 20060608, 383 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA,
 BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC,
 EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG,
 KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN,
 MW, MX, MY, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
 SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
 ZA; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA,
 GB, GR, IE, IS, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR.
 (English). CODEN: PIXXD2. APPLICATION: WO 2005-US43281 20051201.
 PRIORITY: US 2004-633106P 20041203.

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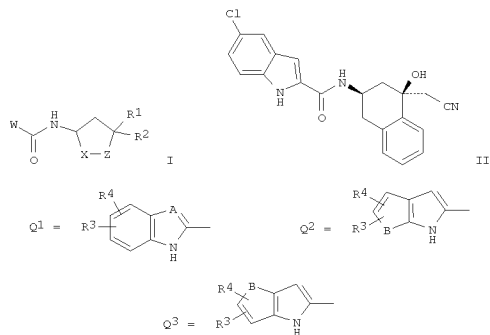
AB Comps. of formula I or pharmaceutically acceptable salts, solvates, or
 esters thereof, are useful in treating diseases or conditions mediated by
 CB1 receptors, such as metabolic syndrome and obesity, neuroinflammatory
 disorders, cognitive disorders and psychosis, addiction (e.g., smoking
 cessation), gastrointestinal disorders, and cardiovascular conditions.
 Comps. of formula I wherein Ar1 and Ar2 are independently
 (un)substituted
 (hetero)aryl; n and m are independently 0 or 1; A is CO, SO2, C(=NOH) and
 derivs., or (un)substituted Cl-3 alkyl; B is NH and derivs., CO or
 (un)substituted Cl-2 alkyl; X is H, alkyl, S-alkyl, SO2-(cyclo)alkyl,
 SO2-(hetero)aryl, benzo(hetero)cycloalkyl, benzoheterocycloalkenyl,
 (un)substituted vinyl(hetero)aryl, etc.; R1 is alkyl, haloalkyl,

L25 ANSWER 15 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 alkenyl-NH2 and derivs., alkylene-OH and derivs., alkylene-N3,
 alkylene-CN, or alkylene-OSO2-alkyl; or two adjacent R1 on the same ring
 carbon atom for a carbonyl group; y is 0, 1, 2, 3, or 4; and their
 pharmaceutically acceptable salts, solvates and esters thereof are
 claimed. Example compd. II (R = Bn) was prepd. by regioselective ring
 cleavage of 4-chlorostyrene oxide with N-methylaminoethanol; the
 resulting
 N-(2-hydroxyethyl)-N-methyl-1-(4-chlorophenyl)-2-amino-1-ethanol
 underwent
 chlorination to give N-(2-chloroethyl)-N-methyl-2-(4-chlorophenyl)-2-
 chloroethylamine which underwent cyclization with 2,4-dichloroaniline to
 give compd. II (R = Me), which underwent demethylation to give II (R =
 H),
 which underwent reductive amination with benzaldehyde to give compd. II
 (R = Bn). All the invention comps. were evaluated for their cannabinoid
 antagonistic activity.
 IT 890031-63-7P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (drug candidate; preparation of substituted piperazines as CB1
 antagonists
 useful for treatment of metabolic disorders)
 RN 890031-63-7 CAPLUS
 CN Methanone, [3-(4-chlorophenyl)-4-(2,4-dichlorophenyl)-1-
 piperazinyl](1,2,3,4-tetrahydro-2-naphthalenyl)- (CA INDEX NAME)



L25 ANSWER 16 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2006:493904 Document No. 145:80230 Preparation of heteroaroylaminotetralins
 and related compounds as glycogen phosphorylase inhibitors. Sher, Philip
 M.; Nirschl, Alexandra A.; Meng, Wei; Washburn, William N. (Bristol-Myers
 Squibb Company, USA). U.S. Pat. Appl. Publ. US 2006011338 A1 20060525,
 42 pp. (English). CODEN: USXXCO. APPLICATION: US 2005-272845 20051114.
 PRIORITY: US 2004-628063P 20041115.

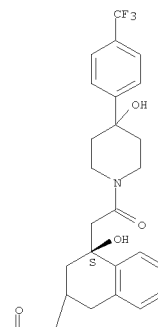
GI



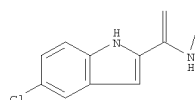
AB Title comps. [I; W = Q1-Q3; X = CH2, CH2CH2, CH2O; Z = (substituted)
 1,2-arylene, 1,2-heteroarylene; R1, R2 = H, (substituted) alkyl, aryl,
 alkyl, heteroaralkyl, alkenyl, cyano, etc.; R3, R4 = H, halo, CF3,
 cyano, alkyl, alkoxy], were prepared. Thus, title compound (II) was
 prepared in
 9 steps from di-Et benzylmalonate, Et chloroacetate, acetonitrile, and
 5-chloroindole-2-carboxylic acid. I deemed to possess activity as
 inhibitors of glycogen phosphorylase demonstrate IC50 of ≤10 μM.
 IT 887752-74-1P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (claimed compound; preparation of heteroaroylaminotetralins and
 related
 comps. as glycogen phosphorylase inhibitors)
 RN 887752-74-1 CAPLUS
 CN 1H-Indole-2-carboxamide, 5-chloro-N-[(4S)-1,2,3,4-tetrahydro-4-hydroxy-4-
 [2-[4-hydroxy-4-[4-(trifluoromethyl)phenyl]-1-piperidinyl]-2-oxoethyl]-2-
 naphthalenyl]- (CA INDEX NAME)

Absolute stereochemistry.

L25 ANSWER 16 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 PAGE 1-A

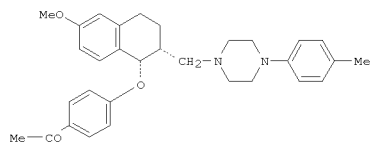


PAGE 2-A



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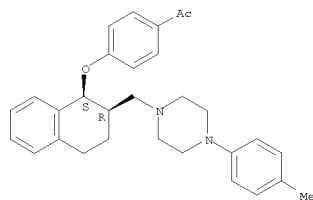
L25 ANSWER 17 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 2006:228532 Document No. 144:4251110 Synthesis and appetite suppressant activity of 1-aryloxy-2-substituted aminomethyltetrahydronaphthalenes as conformationally rigid analogs of fluoxetine. Bhandari, Kalpana; Srivastava, Shipra; Shankar, Giriya; Nath, Chandishwar (Medicinal and Process Chemistry Division, Central Drug Research Institute, Lucknow, 226001, India). Bioorganic & Medicinal Chemistry, 14(8), 2535-2544 (English) 2006. CODEN: BMECEP. ISSN: 0968-0896. OTHER SOURCES: CASREACT 144:425111. Publisher: Elsevier B.V..
 GI



I

AB Several 1-aryloxy-2-substituted aminomethyltetrahydronaphthalenes as conformationally rigid analogs of fluoxetine were synthesized and evaluated for their anorexigenic and antidepressant activities. For SAR studies the related acyclic analogs were also prepared. Out of the 21 synthesized compds., 10 compds. exhibited significant anorexigenic activity (at 75 mmol/kg). Interestingly, all the compds. were devoid of antidepressant effect, except for 2 in which the antidepressant activity was retained. Compound I emerged as the most active compound of the series with better anorexigenic activity (97.92%) compared to fluoxetine (76.25%) and even with a clin. used drug sibutramine, thus providing a new structural lead for appetite suppressants.
 IT 885100-79-8P 885100-81-2P 885100-83-4P
 885100-85-6P 885100-97-0P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (appetite suppressant activity of 1-aryloxy-2-substituted aminomethyltetrahydronaphthalenes)
 RN 885100-79-8 CAPLUS
 CN Piperazine, 1-(4-methylphenyl)-4-[[[(1R,2S)-1,2,3,4-tetrahydro-1-[4-(trifluoromethyl)phenoxy]-2-naphthalenyl]methyl]-, ethanedioate (1:2), rel- (CA INDEX NAME)

L25 ANSWER 17 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 2

CRN 144-62-7
 CMF C2 H2 O4

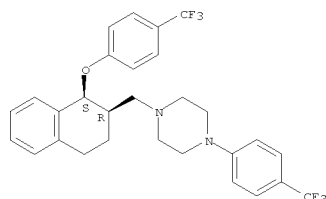


RN 885100-83-4 CAPLUS
 CN Piperazine, 1-[[[(1R,2S)-1,2,3,4-tetrahydro-1-[4-(trifluoromethyl)phenoxy]-2-naphthalenyl]methyl]-4-[4-(trifluoromethyl)phenyl]-, ethanedioate (1:2), rel- (CA INDEX NAME)

CM 1

CRN 885100-82-3
 CMF C29 H28 F6 N2 O

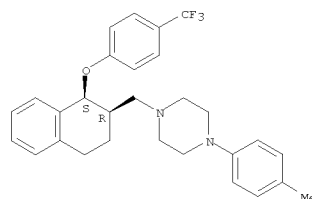
Relative stereochemistry.



L25 ANSWER 17 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 CM 1

CRN 885100-78-7
 CMF C29 H31 F3 N2 O

Relative stereochemistry.



CM 2

CRN 144-62-7
 CMF C2 H2 O4



RN 885100-81-2 CAPLUS
 CN Ethanone, 1-[4-[[[(1R,2S)-1,2,3,4-tetrahydro-2-[[4-(4-methylphenyl)-1-piperazinyl]methyl]-1-naphthalenyl]oxy]phenyl]-, ethanedioate (1:2), rel- (CA INDEX NAME)

CM 1

CRN 885100-80-1
 CMF C30 H34 N2 O2

Relative stereochemistry.

L25 ANSWER 17 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CM 2

CRN 144-62-7
 CMF C2 H2 O4

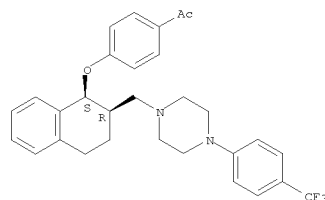


RN 885100-85-6 CAPLUS
 CN Ethanone, 1-[4-[[[(1R,2S)-1,2,3,4-tetrahydro-2-[[4-(4-(trifluoromethyl)phenyl)-1-piperazinyl]methyl]-1-naphthalenyl]oxy]phenyl]-, ethanedioate (1:2), rel- (CA INDEX NAME)

CM 1

CRN 885100-84-5
 CMF C30 H31 F3 N2 O2

Relative stereochemistry.



CM 2

CRN 144-62-7
 CMF C2 H2 O4



RN 885100-97-0 CAPLUS
 CN Ethanone, 1-[4-[[[(1R,2S)-1,2,3,4-tetrahydro-6-methoxy-2-[[4-(4-methylphenyl)-1-piperazinyl]methyl]-1-naphthalenyl]oxy]phenyl]-, ethanedioate (1:2), rel- (CA INDEX NAME)

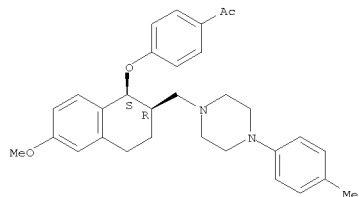
CM 1

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L25 ANSWER 17 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CRN 885100-96-9
CMF C31 H36 N2 O3

Relative stereochemistry.

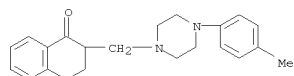


CM 2

CRN 144-62-7
CMF C2 H2 O4

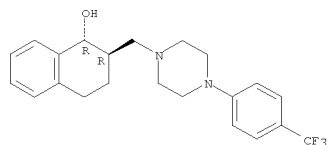


IT 885101-13-3P 885101-14-4P 885101-15-5P
885101-17-7P 885101-18-8P 885101-21-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(appetite suppressant activity of 1-aryloxy-2-substituted aminomethyltetrahydronaphthalenes)
RN 885101-13-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-(4-methylphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



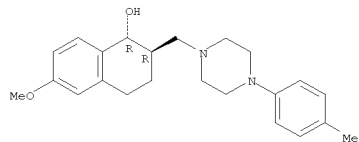
RN 885101-14-4 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-(4-(trifluoromethyl)phenyl)-1-

L25 ANSWER 17 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

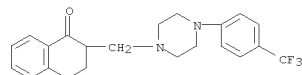


RN 885101-21-3 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-methoxy-2-[[4-(4-methylphenyl)-1-piperazinyl]methyl]-, (1R,2R)-rel- (CA INDEX NAME)

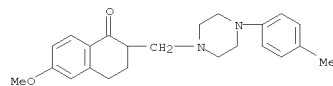
Relative stereochemistry.



L25 ANSWER 17 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
piperazinyl]methyl]- (CA INDEX NAME)

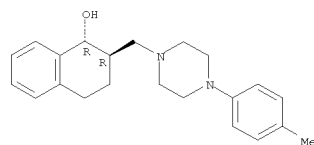


RN 885101-15-5 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[[4-(4-methylphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



RN 885101-17-7 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-2-[[4-(4-methylphenyl)-1-piperazinyl]methyl]-, (1R,2R)-rel- (CA INDEX NAME)

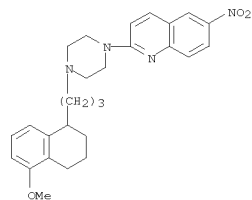
Relative stereochemistry.



RN 885101-18-8 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-2-[[4-[4-(trifluoromethyl)phenyl]-1-piperazinyl]methyl]-, (1R,2R)-rel- (CA INDEX NAME)

Relative stereochemistry.

L25 ANSWER 18 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2005:1143268 Document No. 144:638740 Design and synthesis of long-chain arylpiperazines with mixed affinity for serotonin transporter (SERT) and 5-HT1A receptor. Perrone, Roberto; Berardi, Francesco; Colabufo, Nicola A.; Lacivita, Enza; Larizza, Carmela; Leopoldo, Marcello; Tortorella, Vincenzo (Dipartimento Farmaco-Chimico, Universita degli Studi di Bari, Bari, 70125, Italy). Journal of Pharmacy and Pharmacology, 57(10), 1319-1327 (English) 2005. CODEN: JPPMAB. ISSN: 0022-3573. OTHER SOURCES: CASREACT 144:63874. Publisher: Pharmaceutical Press.
AB A new generation of antidepressant agents could be represented by compds. with mixed activity as serotonin transporter (SERT) inhibitors and 5-HT1A receptor antagonists. We report here on the synthesis and evaluation of SERT and 5-HT1A receptor affinity of long-chain arylpiperazines obtained either by modifying 6-nitroquipazine into a long-chain arylpiperazine or by inserting a modified 6-nitroquipazine moiety or other structures endowed with SERT affinity into a long-chain arylpiperazine with 5-HT1A affinity. Among the compds. studied, 2-[4-(2-methoxyphenyl)piperazin-1-yl]-N-(6-nitro-2-quinolyl)ethylamine (21) and 1-(5-bromo-1,2,3,4-tetrahydronaphthalen-1-yl)-3-[4-(2-methoxyphenyl)-piperazin-1-yl]-1-propanone (24) showed good affinity values for SERT and 5-HT1A receptors (SERT: Ki (inhibition constant) = 71.8 and 62.8 nM; 5-HT1A Ki = 14.2 and 0.82 nM, resp.).
IT 871739-13-8P 871739-14-9P 871739-15-0P
871739-16-1P 871739-24-1P 871739-25-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(aryl)piperazines with mixed affinity for serotonin transporter and 5-HT1A receptor
RN 871739-13-8 CAPLUS
CN Quinoline, 6-nitro-2-[4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]-1-piperazinyl]-, hydrochloride (1:2) (CA INDEX NAME)

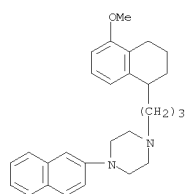


● 2 HCl

RN 871739-14-9 CAPLUS
CN Piperazine, 1-(2-naphthalenyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]-, hydrochloride (1:2) (CA INDEX NAME)

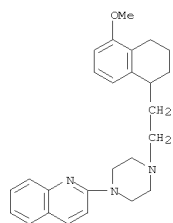
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L25 ANSWER 18 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



●2 HCl

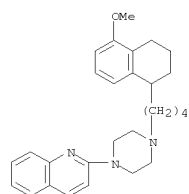
RN 871739-15-0 CAPLUS
CN Quinoline, 2-[4-[2-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)ethyl]-1-piperazinyl]-, hydrochloride (1:3) (CA INDEX NAME)



●3 HCl

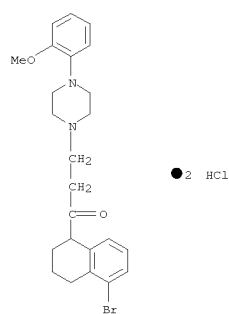
RN 871739-16-1 CAPLUS
CN Quinoline, 2-[4-[4-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)butyl]-1-piperazinyl]-, hydrochloride (1:2) (CA INDEX NAME)

L25 ANSWER 18 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



●2 HCl

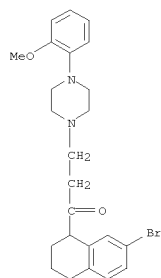
RN 871739-24-1 CAPLUS
CN 1-Propanone, 1-(5-bromo-1,2,3,4-tetrahydro-1-naphthalenyl)-3-[4-(2-methoxyphenyl)-1-piperazinyl]-, hydrochloride (1:2) (CA INDEX NAME)



●2 HCl

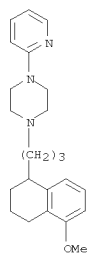
RN 871739-25-2 CAPLUS
CN 1-Propanone, 1-(7-bromo-1,2,3,4-tetrahydro-1-naphthalenyl)-3-[4-(2-methoxyphenyl)-1-piperazinyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 18 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



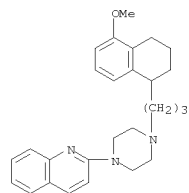
● HCl

IT 154744-88-4 763071-99-4
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(arylpiperazines with mixed affinity for serotonin transporter and 5-HT1A receptor)
RN 154744-88-4 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)



RN 763071-99-4 CAPLUS
CN Quinoline, 2-[4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]-1-piperazinyl]- (CA INDEX NAME)

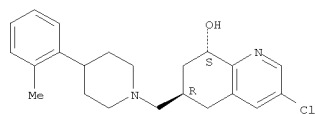
L25 ANSWER 18 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



Relative stereochemistry.

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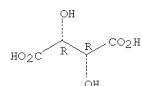
L25 ANSWER 19 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 2

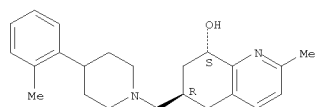
CRN 87-69-4
CMP C4 H6 O6

Absolute stereochemistry.



RN 864829-31-2 CAPLUS
CN 8-Quinololinol, 5,6,7,8-tetrahydro-2-methyl-6-[[4-(2-methylphenyl)-1-piperidinyl]methyl]-, (6R,8S)-rel- (CA INDEX NAME)

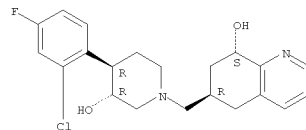
Relative stereochemistry.



RN 864830-99-9 CAPLUS
CN 8-Quinololinol, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-piperidinyl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)- (CA INDEX NAME)

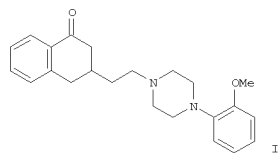
Absolute stereochemistry.

L25 ANSWER 19 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



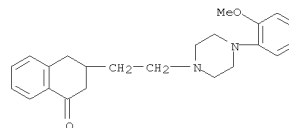
L25 ANSWER 20 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2005:511376 Document No. 143:1937740 Synthesis and binding affinity of novel 3-aminoethyl-1-tetralones, potential atypical antipsychotics. Alvarado, Mario; Coelho, Alberto; Masaquer, Christian F.; Ravina, Enrique; Brea, Jose; Padin, J. Fernando; Loza, Maria I. (Facultad de Farmacia, Departamento de Quimica Organica, Laboratorio de Quimica Farmaceutica, Universidad de Santiago de Compostela, Santiago de Compostela, E-15782, Spain). Bioorganic & Medicinal Chemistry Letters, 15(12), 3063-3066 (English) 2005. CODEN: BMCLE8. ISSN: 0960-894X. OTHER SOURCES: CASREACT 143:193774. Publisher: Elsevier B.V..

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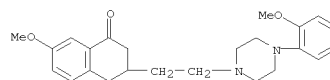


AB A series of 3-aminoethyl-1-tetralones, e.g., I, conformationally constrained higher homologs of haloperidol (standard for typical antipsychotic profile), have been obtained by a four-step route from valerolactone. Their binding affinities at dopamine D2 and serotonin 5-HT2A and 5-HT2C receptors were determined, showing in some cases an atypical antipsychotic profile.
IT 861804-06-0P 861804-07-1P 861804-08-2P
861804-09-3P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation, dopamine D2, serotonin 5-HT2A and 5HT2C binding affinities, antipsychotic activity, and structure-activity relationship of aminoethyltetralones using amination and cyclization as the key steps)
RN 861804-06-0 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[2-[4-(2-methoxyphenyl)-1-piperazinyl]ethyl]- (CA INDEX NAME)

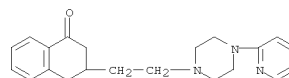
L25 ANSWER 20 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



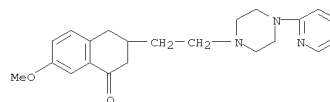
RN 861804-07-1 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-7-methoxy-3-[2-[4-(2-methoxyphenyl)-1-piperazinyl]ethyl]- (CA INDEX NAME)



RN 861804-08-2 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[2-[4-(2-pyridinyl)-1-piperazinyl]ethyl]- (CA INDEX NAME)



RN 861804-09-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-7-methoxy-3-[2-[4-(2-pyridinyl)-1-piperazinyl]ethyl]- (CA INDEX NAME)



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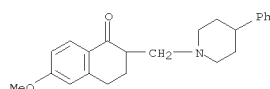
L25 ANSWER 21 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2005:506114 Document No. 143:188544 Characterization of binding site of closed-state KCNQ1 potassium channel by homology modeling, molecular docking, and pharmacophore identification. Du, Lue-Pei; Li, Min-Yong; Tsai, Keng-Chang; You, Qi-Dong; Xia, Lin (Department of Medicinal Chemistry, China Pharmaceutical University, Nanjing, 210009, Peop. Rep. China). Biochemical and Biophysical Research Communications, 332(3), 677-687 (English) 2005. CODEN: BBRCA9. ISSN: 0006-291X. Publisher: Elsevier.

AB This investigation was performed to assess the importance of interaction in the binding of blockers to KCNQ1 potassium using mol. modeling. This work could be considered made up by three main steps: (1) the construction of closed-state structure of KCNQ1 through homol. modeling; (2) the automated docking of three blockers: IKS-142, L-735821, and BMS-1KS, using DOCK program; (3) the generation and validation of pharmacophore for KCNQ1 ligands using Catalyst/HypoGen. The obtained results highlight the hydrophobic or aromatic residues involved in S6 transmembrane domain and the base of the pore helix of KCNQ1, confirming the mutagenesis data and pharmacophore model, and giving new suggestions for the rational design of novel KCNQ1 ligands.

IT 109132-88-9, SQ 23791
 RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
 (homol. modeling, mol. docking, and pharmacophore identification)

permit characterization of binding site of closed-state human KCNQ1 potassium channel)

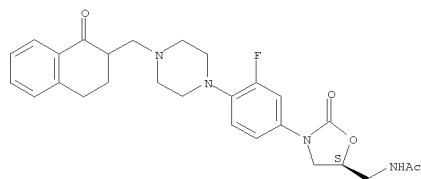
RN 109132-88-9 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[(4-phenyl-1-piperidinyl)methyl]- (CA INDEX NAME)



L25 ANSWER 22 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

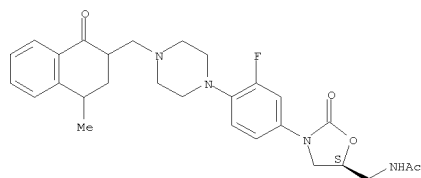
RN 612055-28-4 CAPLUS
 CN Acetamide, N-[[[(5S)-3-[3-fluoro-4-[4-[(1,2,3,4-tetrahydro-1-oxo-2-naphthalenyl)methyl]-1-piperazinyl]phenyl]-2-oxo-5-oxazolidinyl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 612055-32-0 CAPLUS
 CN Acetamide,
 N-[[[(5S)-3-[3-fluoro-4-[4-[(1,2,3,4-tetrahydro-4-methyl-1-oxo-2-naphthalenyl)methyl]-1-piperazinyl]phenyl]-2-oxo-5-oxazolidinyl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

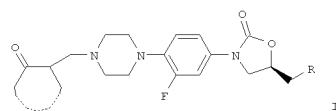


RN 612056-68-5 CAPLUS
 CN Ethanethioamide,
 N-[[[(5S)-3-[3-fluoro-4-[4-[(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-piperazinyl]phenyl]-2-oxo-5-oxazolidinyl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

L25 ANSWER 22 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2004:881223 Document No. 142:713960 Novel Mannich ketones of oxazolidinones as antibacterial agents. Srivastava, Brijesh Kumar; Kapadnis, Prashant B.; Pandya, Purvi; Lohray, Vidya Bhushan (Zydus Research Centre, Ahmedabad, Moraiya, 382210, India). European Journal of Medicinal Chemistry, 39(11), 989-992 (English) 2004. CODEN: EJMCA5. ISSN: 0223-5234. OTHER SOURCES: CASREACT 142:71396. Publisher: Elsevier Ltd..

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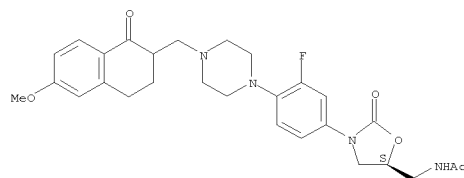


AB A few Mannich ketones of piperazinyl oxazolidinone derivs. were synthesized and their antibacterial activity in various Gram-pos. organisms, such as Bacillus subtilis, Staphylococcus aureus, Staphylococcus epidermidis, and Enterococcus faecalis were evaluated by MIC determination Compound I showed comparable activity to linezolid and superior to eperezolid.

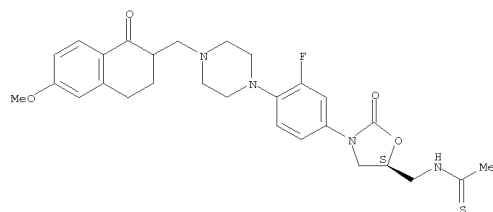
IT 612055-27-3P 612055-28-4P 612055-32-0P
 612056-68-5P
 RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (novel Mannich ketones of oxazolidinones as antibacterial agents)

RN 612055-27-3 CAPLUS
 CN Acetamide,
 N-[[[(5S)-3-[3-fluoro-4-[4-[(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-piperazinyl]phenyl]-2-oxo-5-oxazolidinyl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.



L25 ANSWER 22 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



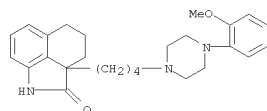
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L25 ANSWER 23 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2004:534173 Document No. 141:890160 Preparation of
 benzimidazolylazabicyclooctylethylpiperidines as Ccr5 antagonists for the
 treatment of HIV infection. Kazmierski, Wieslaw Mieczyslaw; Aquino,
 Christopher Joseph; Bifulco, Neil; Boros, Eric Eugene; Chauder, Brian
 Andrew; Chong, Pek Yoke; Duan, Maosheng; Deanda, Felix, Jr.; Koble,
 Cecilia Suarez; McLean, Ed Williams; Peckham, Jennifer Poole; Perkins,
 Angilique C.; Thompson, James Benjamin; Vanderwall, Dana (Smithkline
 Beecham Corporation, USA; et al.; et al.). PCT Int. Appl. WO 2004054974
 A2 20040701, 859 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ,
 BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ,
 EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE,
 KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX,
 MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT,
 BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE,
 IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN:
 FIKXD2. APPLICATION: WO 2003-US39644 20031212. PRIORITY: US
 2002-433634P
 20021213.
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

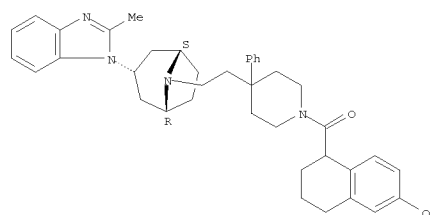
AB Comps. I [R1 = (optionally substituted) alkyl, aryl, heteroaryl,
 carbocyclyl; R2 = H, (optionally substituted) alkyl, aryl, heteroaryl,
 cycloalkyl, heterocycloalkyl, aralkyl, heteroarylalkyl,
 heteroarylalkyl, heteroarylalkyl, heteroarylalkyl; R3 = H, halo,
 cyano, trifluoromethyl, (optionally substituted) amino, acylamino, alkyl;
 X = Cl-5 alkylene, optionally substituted with oxo or thioxo groups or
 halogen atoms, and optionally containing 1-3 oxygen, nitrogen, sulfur, or
 phosphorus atoms; Y = carbonyl, thiocarbonyl, 1,2-dioxoethylene,
 oxyalkylcarbonyl, sulfinyl, sulfonyl, oxycyanoinmino, (optionally
 substituted) aminocarbonyl, carbonylamino, aminothiocarbonyl,
 oximinomethyl, thioiminomethyl, amino(cyanoinmino)methyl,
 (cyanoinmino)methyl, amino(acylimino)methyl, amino(sulfonylimino)methyl,
 amino(sulfinylimino)methyl, amino(alkoxyimino)methyl, amino(imino)methyl,
 (cyanoinmino)methoxy, iminomethoxy, (cyanoinmino)methanethiyl,
 alkylcarbonyloxy; A = saturated, partially saturated, or aromatic
 monocyclic ring
 with 5-6 atoms or a bicyclic ring with 8-10 members containing 0-5
 nitrogen,
 oxygen, and/or sulfur atoms] such as II are prepared I are prepared as
 Ccr5
 antagonists for the treatment of viral infections, (particularly HIV
 infection), related syndromes such as AIDS-related complex (ARC),
 progressive generalized lymphadenopathy, Kaposi's sarcoma, and neurol.
 conditions, and other diseases such as multiple sclerosis, rheumatoid
 arthritis, Crohn's disease, and immune-mediated disorders. The invention
 compts. have PIC50 values of ≥ 5 in assays for Ccr5 antagonism.
 Piperidineacetaldehyde III is prepared in four steps from
 4-phenyl-4-piperidinecarbonitrile by protection of the piperidine with
 Boc

L25 ANSWER 24 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2004:263486 Document No. 140:417259 Studies on 1-arylpiperazine derivatives
 with affinity for rat 5-HT7 and 5-HT1A receptors. Leopoldo, Marcello;
 Berardi, Francesco; Colabufio, Nicola A.; Contino, Marialessandra;
 Lacivita, Enza; Perone, Roberto; Tortorella, Vincenzo (Dipartimento
 Farmaco-Chimico, Università degli Studi di Bari, Bari, 70125, Italy).
 Journal of Pharmacy and Pharmacology, 56(2), 247-255 (English) 2004.
 CODEN: JPPMAB. ISSN: 0022-3573. Publisher: Pharmaceutical Press.
 AB Several 1-aryl-4-(2-arylethyl)piperazine derivs. were synthesized and
 tested in-vitro for their binding affinity for 5-HT7 and 5-HT1A
 receptors.
 These compts. displayed 5-HT7 receptor affinity ranging between $K_i=474$ nM
 and $K_i=8.2$ nM, besides high affinity for the 5-HT1A receptor. Intrinsic
 activity of the most potent compts. was assessed.
 4-[2-(3-Methoxyphenyl)ethyl]-1-(2-methoxyphenyl)piperazine (16) and
 1-(1,2-benzisoxazol-3-yl)-4-[2-(3-methoxyphenyl)ethyl]piperazine (20)
 ($K_i=24.5$ and 8.2 nM, resp.) behaved as partial agonist and full agonist,
 resp., when tested for 5-HT7 receptor-mediated relaxation of substance
 P-induced guinea-pig ileum contraction.
 IT 201608-39-1
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (arylpiperazine derivs. with affinity for rat 5-HT7 and 5-HT1A
 receptors)
 RN 201608-39-1 CAPLUS
 CN Benz[cd]indol-2(1H)-one,
 2a,3,4,5-tetrahydro-2a-[4-[4-(2-methoxyphenyl)-1-
 piperazinyl]butyl]- (CA INDEX NAME)

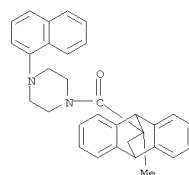


L25 ANSWER 23 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 anhydride, redn. of the nitrile with diisobutylaluminum hydride, Wittig
 olefination with methoxymethylphosphonium chloride, and hydrolysis of the
 enol ether with catalytic p-toluenesulfonic acid monohydrate. The
 hydrochloride of endo-(benzimidazolyl)azabicyclooctane IV is prep'd. in
 five steps from tert-Bu
 endo-3-oxo-8-azabicyclo[3.2.1]octane-8-carboxylate;
 reductive amination with benzylamine, reductive cleavage of the benzyl
 group by palladium-mediated hydrogenation, a nucleophilic aryl
 substitution reaction with 1-fluoro-2-nitrobenzene, redn. of the nitro
 group by hydrogenation over palladium on carbon, and treatment with
 tri-Et
 orthoacetate followed by treatment with hydrochloric acid in ethanol.
 Coupling of III and IV by reductive amination with sodium
 triacetoxymethylborohydride, cleavage of the Boc group with hydrochloric acid
 in
 dioxane, and acylation with pivaloyl chloride and triethylamine yields
 II.
 IT 716354-57-3P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (drug candidate; preparation of
 benzimidazolylazabicyclooctylethylpiperidine
 Ccr5 antagonists in treatment of bacterial and viral infections and
 other diseases)
 RN 716354-57-3 CAPLUS
 CN Methanone, [4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-
 azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenyl-1-piperidinyl][1,2,3,4-
 tetrahydro-6-hydroxy-1-naphthalenyl]- (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 25 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2004:80449 Document No. 140:157927 Homology modeling of nuclear hormone
 receptor Site II and design of Site II ligands. Doweyko, Arthur; Nadler,
 Steven G. (Bristol-Myers Squibb Company, USA). PCT Int. Appl. WO
 2004009016 A2 20040129, 276 pp. DESIGNATED STATES: W: AE, AG, AL, AM,
 AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK,
 DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,
 KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW,
 MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL,
 SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE,
 DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN,
 TD, TG, TR. (English). CODEN: FIKXD2. APPLICATION: WO 2003-US22299
 20030717. PRIORITY: US 2002-396907P 20020718.
 AB A binding site in nuclear hormone receptors is described and its
 structural coordinates are provided. The invention provides
 machine-readable data storage media comprising structure coordinates of
 Site II and computer systems comprising the machine-readable data storage
 media. The invention provides methods used in the design and
 identification of ligands of Site II and of modulators of nuclear hormone
 receptors. The invention provides ligands of Site II, modulators of
 NHRs,
 pharmaceutical compts. comprising modulators of NHRs, methods of
 modulating NHRs, and methods of treating diseases by administering
 modulators of an NHR. Also provided are methods of designing mutants,
 mutant NHRs, Site II binding assays, and models of Site II.
 IT 650625-50-6P
 RL: CPS (Chemical process); PAC (Pharmacological activity); PEP
 (Physical,
 engineering or chemical process); SPN (Synthetic preparation); BIOL
 (Biological study); PREP (Preparation); PROC (Process)
 (homol. modeling of nuclear hormone receptor Site II in ligand binding
 domain and design of Site II ligands)
 RN 650625-50-6 CAPLUS
 CN Methanone, (9,10-dihydro-11-methyl-9,10-ethanoanthracen-11-yl)[4-(1-
 naphthalenyl)-1-piperazinyl]- (CA INDEX NAME)



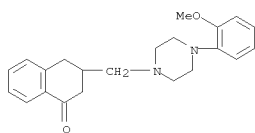
10590585.trn

L25 ANSWER 26 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2004:51780 Document No. 140:2871550 Chemoenzymatic synthesis and binding affinity of novel (R)- and (S)-3-aminomethyl-1-tetralones, potential atypical antipsychotics. Caro, Yolanda; Torrado, Maria; Masaguer, Christian F.; Ravina, Enrique; Padin, Fernando; Brea, Jose; Loza, Maria

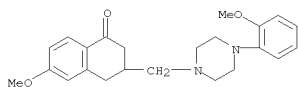
I. (Facultad de Farmacia, Laboratorio de Quimica Farmaceutica (Drug Research & Development Group), Departamento de Quimica Organica, Universidad de Santiago de Compostela, Santiago de Compostela, E-15782, Spain). Bioorganic & Medicinal Chemistry Letters, 14(3), 585-589 (English) 2004. CODEN: BMCLE8. ISSN: 0960-894X. OTHER SOURCES: CASREACT 140:287155. Publisher: Elsevier Science B.V..

AB A series of (R)- and (S)-3-aminomethyl-1-tetralones, conformationally constrained analogs of haloperidol, have been obtained by enzymic resolution of the corresponding racemic 3-hydroxymethyl-1-tetralones using Pseudomonas fluorescens lipase. Their binding affinities at dopamine D2 and serotonin 5-HT2A and 5-HT2C receptors were determined showing in some cases an atypical antipsychotic profile with Meltzer's ratio higher than 1.30. IT 133496-60-3P 676139-10-9P 676139-11-0P 676139-12-1P 676139-13-2P 676139-14-3P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (chemoenzymic synthesis of (R)- and (S)-3-aminomethyl-1-tetralones and their binding affinities at dopamine D2 and serotonin 5-HT2A and

5-HT2C receptors)
RN 133496-60-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



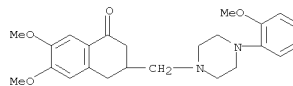
RN 676139-10-9 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-3-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



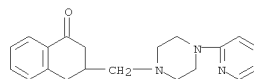
L25 ANSWER 26 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

L25 ANSWER 26 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

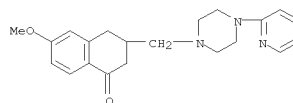
RN 676139-11-0 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6,7-dimethoxy-3-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



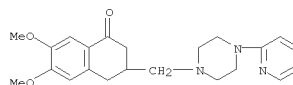
RN 676139-12-1 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[[4-(2-pyridinyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



RN 676139-13-2 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-3-[[4-(2-pyridinyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



RN 676139-14-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6,7-dimethoxy-3-[[4-(2-pyridinyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



L25 ANSWER 27 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2003:981457 Document No. 140:2284530 Tetrahydronaphthalene-derived amino alcohols and amino ketones as potent and selective inhibitors of the delayed rectifier potassium current (IKr). Ahmad, Saleem; Doweiko, Lidia; Ashfaq, Aaila; Ferrara, Francis N.; Bisaha, Sharon N.; Schmidt, Joan B.; DiMarco, John; Conder, Mary Lee; Jenkins-West, Tonya; Normandin, Diane E.;

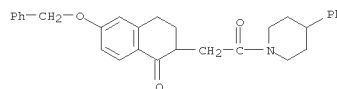
Russell, Anita D.; Smith, Mark A.; Levesque, Paul C.; Lodge, Nicholas J.; Lloyd, John; Stein, Philip D.; Atwal, Karnail S. (Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, NJ, 08543, USA).

Bioorganic & Medicinal Chemistry Letters, 14(1), 99-102 (English) 2004. CODEN: BMCLE8. ISSN: 0960-894X. OTHER SOURCES: CASREACT 140:228453. Publisher: Elsevier Science B.V..

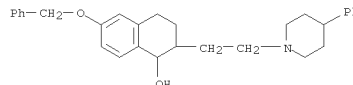
AB Class III anti-arrhythmic drugs (e.g., dofetilide) prolong cardiac action potential duration (APD) by blocking the fast component of the delayed rectifier potassium current (IKr). The block of IKr can result in life threatening ventricular arrhythmias (i.e., torsades de pointes). Unlike IKr, the role of the slow component of the delayed rectifier potassium current (IKs) becomes significant only at faster heart rate. Therefore selective blockers of IKs could prolong APD with a reduced propensity to cause pro-arrhythmic side effects. This report describes structure-activity relationships (SARs) of a series of IKs inhibitors derived from 6-alkoxytetralones with good in vitro activity (IC50 ≥ 30 nM) and ≤40-fold IKs/IKr selectivity.

IT 667900-14-3P 667900-19-8P 667900-23-4P RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (tetrahydronaphthalene-derived amino alcs. and amino ketones as potent and selective inhibitors of delayed rectifier potassium current IKs as class III antiarrhythmics)

RN 667900-14-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[2-oxo-2-(4-phenyl-1-piperidinyl)ethyl]-6-(phenylmethoxy)- (CA INDEX NAME)

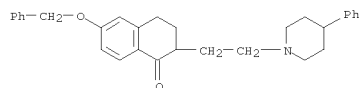


RN 667900-19-8 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-(phenylmethoxy)-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



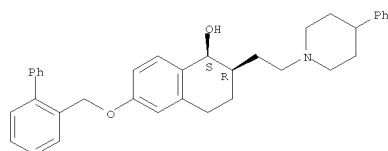
10590585.trn

L25 ANSWER 27 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 RN 667900-23-4 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-(phenylmethoxy)-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

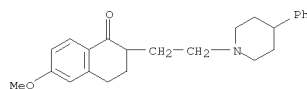


IT 212256-93-4P 212257-25-5P 212257-52-8P
 212257-53-9P 212257-67-5P 667900-24-5P
 667900-25-6P 667900-26-7P 667900-27-8P
 667900-28-9P 667900-32-5P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (tetrahydronaphthalene-derived amino alcs. and amino ketones as potent and selective inhibitors of delayed rectifier potassium current I_{Ks} as class III antiarrhythmics)
 RN 212256-93-4 CAPLUS
 CN 1-Naphthalenol,
 6-([1,1'-biphenyl]-2-ylmethoxy)-1,2,3,4-tetrahydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]-, (1R,2S)-rel- (CA INDEX NAME)

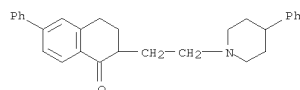
Relative stereochemistry.



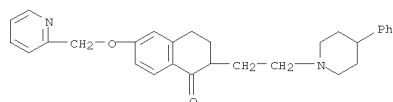
RN 212257-25-5 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



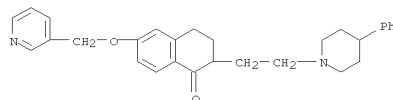
L25 ANSWER 27 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-phenyl-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



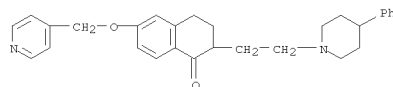
RN 667900-26-7 CAPLUS
 CN 1(2H)-Naphthalenone,
 3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]-6-(2-pyridinylmethoxy)- (CA INDEX NAME)



RN 667900-27-8 CAPLUS
 CN 1(2H)-Naphthalenone,
 3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]-6-(3-pyridinylmethoxy)- (CA INDEX NAME)



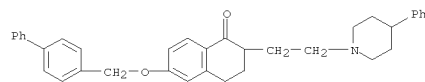
RN 667900-28-9 CAPLUS
 CN 1(2H)-Naphthalenone,
 3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]-6-(4-pyridinylmethoxy)- (CA INDEX NAME)



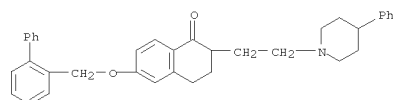
RN 667900-32-5 CAPLUS
 CN 1-Naphthalenol,
 6-([1,1'-biphenyl]-2-ylmethoxy)-1,2,3,4-tetrahydro-2-[2-(4-

L25 ANSWER 27 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

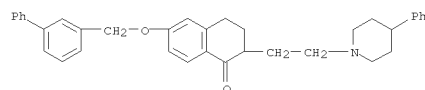
RN 212257-52-8 CAPLUS
 CN 1(2H)-Naphthalenone, 6-([1,1'-biphenyl]-4-ylmethoxy)-3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



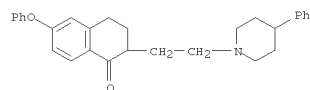
RN 212257-53-9 CAPLUS
 CN 1(2H)-Naphthalenone, 6-([1,1'-biphenyl]-2-ylmethoxy)-3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212257-67-5 CAPLUS
 CN 1(2H)-Naphthalenone, 6-([1,1'-biphenyl]-3-ylmethoxy)-3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



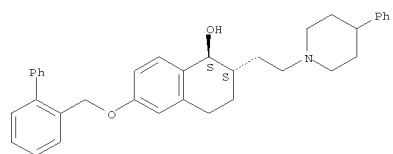
RN 667900-24-5 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-phenoxy-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



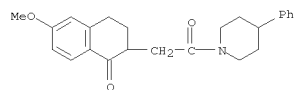
RN 667900-25-6 CAPLUS

L25 ANSWER 27 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 phenyl-1-piperidinyl)ethyl]-, (1R,2R)-rel- (CA INDEX NAME)

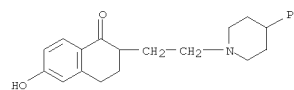
Relative stereochemistry.



IT 212256-71-8P 212259-30-8P 667900-15-4P
 667900-16-5P 667900-17-6P 667900-18-7P
 667900-20-1P 667900-21-2P 667900-22-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (tetrahydronaphthalene-derived amino alcs. and amino ketones as potent and selective inhibitors of delayed rectifier potassium current I_{Ks} as class III antiarrhythmics)
 RN 212256-71-8 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[2-oxo-2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



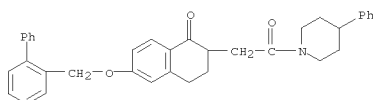
RN 212259-30-8 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-hydroxy-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



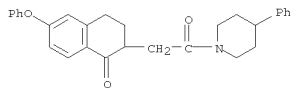
RN 667900-15-4 CAPLUS
 CN 1(2H)-Naphthalenone,
 6-([1,1'-biphenyl]-2-ylmethoxy)-3,4-dihydro-2-[2-oxo-2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

10590585.trn

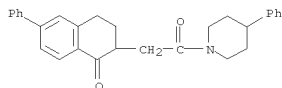
L25 ANSWER 27 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



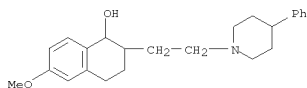
RN 667900-16-5 CAPLUS
CN 1(2H)-Naphthalenone,
3,4-dihydro-2-[2-oxo-2-(4-phenyl-1-piperidinyl)ethyl]-
6-phenoxy- (CA INDEX NAME)



RN 667900-17-6 CAPLUS
CN 1(2H)-Naphthalenone,
3,4-dihydro-2-[2-oxo-2-(4-phenyl-1-piperidinyl)ethyl]-
6-phenyl- (CA INDEX NAME)



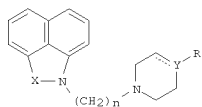
RN 667900-18-7 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-methoxy-2-[2-(4-phenyl-1-
piperidinyl)ethyl]- (CA INDEX NAME)



RN 667900-20-1 CAPLUS
CN 1-Naphthalenol,
6-([1,1'-biphenyl]-2-ylmethoxy)-1,2,3,4-tetrahydro-2-[2-(4-
phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

L25 ANSWER 28 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2003:876891 Document No. 139:3958940 Optimization of the Pharmacophore
Model
for 5-HT7R Antagonism. Design and Synthesis of New Naphtholactam and
Naphthosultam Derivatives. Lopez-Rodriguez, Maria L.; Porras, Esther;
Morcillo, M. Jose; Benhamu, Bellinda; Soto, Luis J.; Lavandera, Jose L.;
Ramos, Jose A.; Olivella, Mireia; Campillo, Mercedes; Pardo, Leonardo
(Departamento de Química Organica I, Facultad de Ciencias Químicas and
Departamento de Bioquímica y Biología Molecular III, Facultad de
Medicina,
Universidad Complutense, Madrid, E-28040, Spain). Journal of Medicinal
Chemistry, 46(26), 5638-5650 (English) 2003. CODEN: JMCMAR. ISSN:
0022-2623. OTHER SOURCES: CASREACT 139:395894. Publisher: American
Chemical Society.

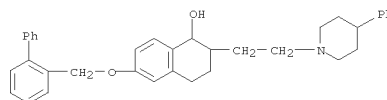
GI



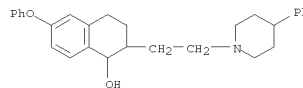
AB An optimization of a preliminary pharmacophore model for 5-HT7R
antagonism, with the incorporation of recently reported ligands and using
an efficient procedure with the CATALYST program is reported. The model
consists of five features: a pos. ionizable atom (PI), a H-bonding
acceptor group (HBA), and three hydrophobic regions (HYD). This model
has been supported by the design, synthesis, and biol. evaluation of new
naphtholactam and naphthosultam derivs. of general structure I (X = CO,
SO₂; Y = N, CH, C; n = 1, 3 - 6; R = H, Me, Me₂CH, cyclohexyl, Ph,
2-MeOC₆H₄). A systematic structure-affinity relationship (SAFIR) study
on these analogs has allowed us to confirm that the model incorporates the
essential structural features for 5-HT7R antagonism. In addition,
computational simulation of the complex between I (X = CO; Y = N, n = 5;
R = Ph) and a rhodopsin-based 3D model of the 5-HT7R transmembrane domain
has permitted us to define the mol. details of the ligand-receptor
interaction and gives addnl. support to the proposed pharmacophore model
for 5-HT7R antagonism: (i) the HBA feature of the pharmacophore model
binds Ser5.42 and Thr5.43, (ii) the HYD1 feature interacts with Phe6.52,
the (iii) the PI feature forms an ionic interaction with Asp3.32, and (iv)
the HYD3 (AR) feature interacts with a set of aromatic residues (Phe3.28,
Tyr7.43). These results provide the tools for the design and synthesis
of new ligands with predetd. affinities and pharmacol. properties.

IT 201608-39-1 201608-45-9 201608-78-8
201608-87-9 201608-88-0 201609-20-3
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL
(Biological study)
(optimization of the pharmacophore model for serotonergic 5-HT7

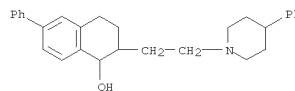
L25 ANSWER 27 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 667900-21-2 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-phenoxy-2-[2-(4-phenyl-1-
piperidinyl)ethyl]- (CA INDEX NAME)

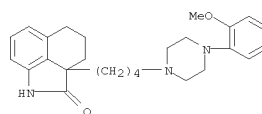


RN 667900-22-3 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-phenyl-2-[2-(4-phenyl-1-
piperidinyl)ethyl]- (CA INDEX NAME)

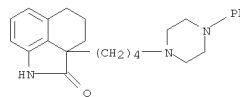


L25 ANSWER 28 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

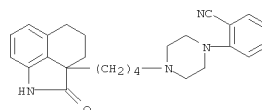
RN 201608-39-1 CAPLUS
CN Benz[cd]indol-2(1H)-one,
2a,3,4,5-tetrahydro-2a-[4-[4-(2-methoxyphenyl)-1-
piperazinyl]butyl]- (CA INDEX NAME)



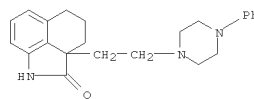
RN 201608-45-9 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-phenyl-1-
piperazinyl)butyl]- (CA INDEX NAME)



RN 201608-78-8 CAPLUS
CN Benzonitrile, 2-[4-[4-(1,2,4,5-tetrahydro-2-oxobenz[cd]indol-2a(3H)-
yl)butyl]-1-piperazinyl]- (CA INDEX NAME)



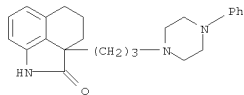
RN 201608-87-9 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[2-(4-phenyl-1-
piperazinyl)ethyl]- (CA INDEX NAME)



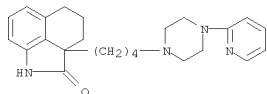
10590585.trn

L25 ANSWER 28 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

RN 201608-88-0 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[3-(4-phenyl-1-piperazinyl)propyl]- (CA INDEX NAME)



RN 201609-20-3 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-pyridinyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



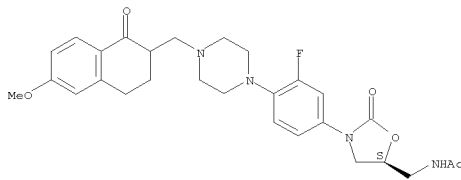
L25 ANSWER 29 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2003:796700 Document No. 139:3077980 Preparation of 3-(4-piperazinophenyl) substituted oxazolidinones as novel anti-infective compounds and pharmaceutical compositions containing them. Lohray, Braj Bhushan; Lohray, Vidya Bhushan; Srivastava, Brijesh Kumar (Cadila Healthcare Limited, India). PCT Int. Appl. WO 2003082864 A2 20031009, 78 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY,

BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2003-IN81 20030326. PRIORITY: IN 2002-MU310 20020401. GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

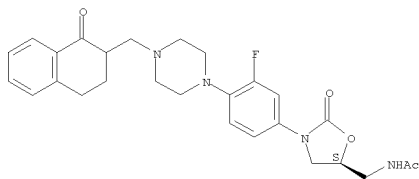
AB The title compds. [I; Ar = (un)substituted Ph, 5-6 membered heteroaryl; R1, R2 = H, halo, alkyl, etc.; Y = II-IV (wherein R3, R4 = H, alkyl, halo, etc.; X = O, S, NR5; R5 = H, alkyl, aryl; A = (un)substituted (un)saturated single or fused ring optionally containing one or more heteroatoms selected from N, S, O; Z = H, alkyl, CN, etc.); W = OH, N3, NH2, NCS, etc.], useful for treating bacterial infections, psoriasis, arthritis, were prepared Thus, amidation of (S)-N-[(3-[3-fluoro-4-(N-piperazinyl)phenyl]-2-oxo-5-oxazolidinyl)methyl]acetamide with 3-(2-thienyl)acrylic acid afforded 53% (S)-V. The compds. I inhibited the growth of bacteria such as Staphylococcus aureus, Staphylococcus epidermidis and Enterococcus faecalis with MIC's in a range of about 0.25 µg/mL to about 64 µg/mL. Pharmaceutical composition comprising the compound I is claimed. IT 612055-27-3P 612055-28-4P 612055-31-9P 612055-32-0P 612056-68-5P 612056-70-9P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 3-(4-piperazinophenyl) substituted oxazolidinones as novel anti-infective compds. and pharmaceutical compns. containing them) RN 612055-27-3 CAPLUS CN Acetamide, N-[[[(5S)-3-[3-fluoro-4-[4-[(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-piperazinyl]phenyl]-2-oxo-5-oxazolidinyl)methyl]- (CA INDEX NAME) Absolute stereochemistry.

L25 ANSWER 29 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 612055-28-4 CAPLUS
CN Acetamide, N-[[[(5S)-3-[3-fluoro-4-[4-[(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-piperazinyl]phenyl]-2-oxo-5-oxazolidinyl)methyl]- (CA INDEX NAME)

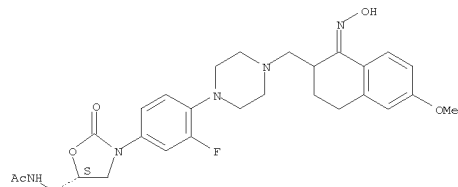
Absolute stereochemistry.



RN 612055-31-9 CAPLUS
CN Acetamide, N-[[[(5S)-3-[3-fluoro-4-[4-[(1,2,3,4-tetrahydro-1-(hydroxyimino)-6-methoxy-2-naphthalenyl)methyl]-1-piperazinyl]phenyl]-2-oxo-5-oxazolidinyl)methyl]- (CA INDEX NAME)

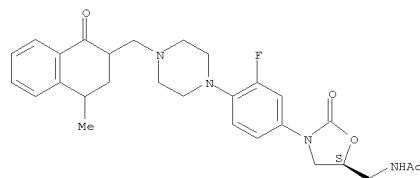
Absolute stereochemistry.
Double bond geometry unknown.

L25 ANSWER 29 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 612055-32-0 CAPLUS
CN Acetamide, N-[[[(5S)-3-[3-fluoro-4-[4-[(1,2,3,4-tetrahydro-4-methyl-1-oxo-2-naphthalenyl)methyl]-1-piperazinyl]phenyl]-2-oxo-5-oxazolidinyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

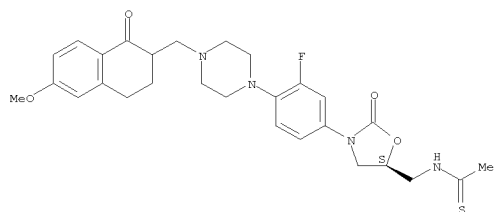


RN 612056-68-5 CAPLUS
CN Ethanethioamide, N-[[[(5S)-3-[3-fluoro-4-[4-[(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-piperazinyl]phenyl]-2-oxo-5-oxazolidinyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

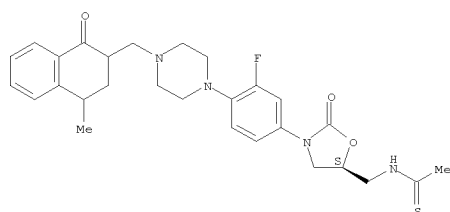
10590585.trn

L25 ANSWER 29 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 612056-70-9 CAPLUS
CN Ethanethioamide,
N-[[[(5S)-3-[3-fluoro-4-[4-[(1,2,3,4-tetrahydro-4-methyl-1-oxo-2-naphthalenyl)methyl]-1-piperazinyl]phenyl]-2-oxo-5-oxazolidinyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



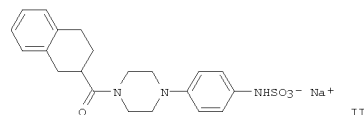
L25 ANSWER 30 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2003:796468 Document No. 139:3076080 Preparation of sodium sulfamic acid salts as inhibitors of human cytoplasmic protein tyrosine phosphatases

for the treatment of wounds and of damaged tissues. Sankar, Sabita; Raheja, Raj K.; Newman, Michael J.; Bhat, Abhijit S.; Slee, Deborah H.; Lee, Kyung

Joo; Lee, Younghee N.; McConnell, Stephen J.; Coats, Eugene A.; Nguyen, Truc; Soll, Richard; Smith, Mark; Short, Kevin M.; Ligsay, Kathleen J. (Ontogen Corporation, USA; et al.). PCT Int. Appl. WO 2003082263 A1 20031009, 110 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2003-US9750 20030328. PRIORITY: US 2002-368901P 20020329; US

2002-431950P
20021209.

GI



AB Sodium sulfamates (RY1)(R1Y1)(R2Y2)X-T-NHSO3-Na+ I [R, R1, R2 = H, (un)substituted alkyl, cycloalkyl, aralkyl, heteroarylalkyl, alkylaryl, alkylheteroaryl, alkylcarboxyalkyl, alkoxyalkyl, arylalkoxyalkyl, heteroarylalkoxyalkyl; R3, R7 = (un)substituted aralkyl, heteroaralkyl, alkyl; R4, R5, R6 = alkyl, aralkyl, heteroaralkyl, R7Y1; T = single bond, NH; X = (un)substituted Ph, pyridyl, pyrimidinyl, furyl, thienyl, indolyl, thiazolyl, imidazolyl, oxazolyl, isoxazolyl; Y1 = single bond, (un)substituted NHC(:O), NHC(:S), O(C(:O), NHC(:O)NH, NHC(:S)NH, NHSO2, NHSO, O, NH; Y2 = (un)substituted NHC(:O), NHC(:S), O(C(:O), NHC(:O)NH, NHC(:S)NH, NHSO2, NHSO, O, NH, O2CCH:CHY1, NHCOC:CHY1, A(CH2/mY1) such

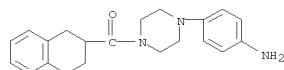
as II are prepared as inhibitors of human cytoplasmic protein tyrosine phosphatase, an enzyme that impedes angiogenesis, for the treatment of wounds and diseased tissue by the acceleration of wound and injury repair; Et N- [4-(4-morpholinyl)phenyl]sulfamate is also claimed as a compound of the invention. Pharmaceutical comps. containing I are also claimed (no data). II is prepared by alkylation of 4-nitrophenylpiperazine with 3-fluorobenzyl bromide followed by reduction of the nitro group to an amino

L25 ANSWER 30 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
group (procedures but no prep. data given); treatment of the aniline with chlorosulfonic acid followed by deprotonation of the sulfamic acid with sodium carbonate yields II. Seventy-six example comps. inhibit human cytoplasmic protein tyrosine phosphatase (EC 3.1.3.2) with IC50 values between 0.06 μ M and 61 μ M. E.g., II inhibits human cytoplasmic protein tyrosine phosphatase with an IC50 value of 0.06 μ M.

IT 611399-62-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediates; preparation of sodium sulfamates and a sulfamic acid ester

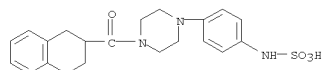
as human cytoplasmic protein tyrosine phosphatase inhibitors for the treatment of wounds and tissue damage by accelerating wound and tissue repair)

RN 611399-62-3 CAPLUS
CN Methanone, [4-(4-aminophenyl)-1-piperazinyl](1,2,3,4-tetrahydro-2-naphthalenyl)- (CA INDEX NAME)



IT 611397-82-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(invention comps.; preparation of sodium sulfamates and a sulfamic acid ester as human cytoplasmic protein tyrosine phosphatase inhibitors for the treatment of wounds and tissue damage by accelerating wound and tissue repair)

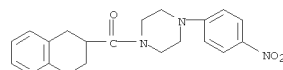
RN 611397-82-1 CAPLUS
CN Sulfamic acid, N-[4-[4-[(1,2,3,4-tetrahydro-2-naphthalenyl)carbonyl]-1-piperazinyl]phenyl]- (CA INDEX NAME)



IT 611401-03-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting materials; preparation of sodium sulfamates and a sulfamic acid ester as human cytoplasmic protein tyrosine phosphatase inhibitors for the treatment of wounds and tissue damage by accelerating wound and tissue repair)

RN 611401-03-7 CAPLUS
CN Methanone, [4-(4-nitrophenyl)-1-piperazinyl](1,2,3,4-tetrahydro-2-naphthalenyl)- (CA INDEX NAME)

L25 ANSWER 30 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



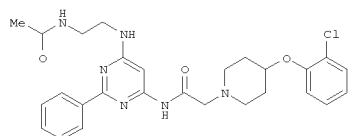
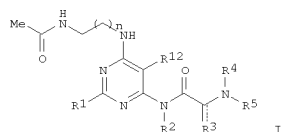
10590585.trn

L25 ANSWER 31 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2003;511098 Document No. 139;853660 Preparation of
N-(pyrimidin-4-yl)acetamides as A2b adenosine receptor selective
antagonists. Castelhana, Arlindo; McKibben, Bryan; Steinig, Arno;
Collington, Eric William (OSI Pharmaceuticals, Inc., USA). PCT Int.

Appl. WO 2003053366 A2 20030703, 150 pp. DESIGNATED STATES: W: AE, AG, AL,
AM,

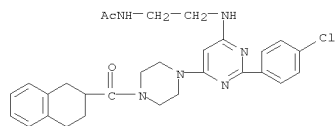
AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK,
DM, DG, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,
KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW,
MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM,
TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF,
BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU,
MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2.
APPLICATION: WO 2002-US41273 20021220. PRIORITY: US 2001-342595P
20011220.

GI



AB Title compds. I [wherein R1 = (un)substituted Ph, heterocyclyl, or
heteroaryl; R2 and R3 = independently H or (un)substituted (cyclo)alkyl,
alkanoyl, alkoxy(carbonyl), alkenyl, monocyclic or bicyclic aryl,
heteroaryl, or heterocyclyl; or R2 and R3 are joined to form a
heterocyclic ring; wherein the dashed line = a double bond which may be
present or absent, and when present R3 = O; R4 and R5 = independently
(un)substituted (cyclo)alkyl, alkanoyl, alkoxy(carbonyl), alkenyl,
monocyclic or bicyclic aryl, heteroaryl, or heterocyclyl; or NR4R5 =
(un)substituted monocyclic or bicycyl, heterocyclyl, or heteroaryl; R12
=

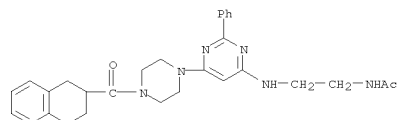
L25 ANSWER 31 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



L25 ANSWER 31 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
H, alkyl, halo, or cyano; n = 0-4; or enantiomers, tautomers, or
pharmaceutically acceptable salts thereof] were prepd. as A2b adenosine
receptor antagonists. For example, cycloadn. of benzamidine•HCl and
di-Et malonate using DBU in DMF gave 2-phenylpyrimidine-4,6-diol (73%).
Chlorination (95%), amination (93%), substitution with
N-(2-aminoethyl)acetamide (57%), and amidation with chloroacetyl chloride
(91%) provided N-[6-(2-acetylaminomethylamino)-2-phenylpyrimidin-4-yl]-2-
chloroacetamide. Coupling of the chloroacetamide with
4-(2-chlorophenoxy)piperidine in the presence of NaI and DIPEA in 3:1
acetonitrile:THF afforded II (86%). Comps. of the invention showed
greater than tenfold selectivity for the human A2b adenosine receptor (Ki
values <100 nM) over the A1, A2a, and A3 receptors in radioligand binding
assays. Thus, I and pharmaceutical compns. comprising I are useful for
the treatment of diseases assocd. with the A2b adenosine receptor, such

as
asthma, diabetes, or proliferating tumors assocd. with mast cell
degranulation (no data).
IT 552871-19-9P, N-[2-[[2-Phenyl-6-[4-[(1,2,3,4-
tetrahydronaphthalen-2-yl)carbonyl]piperazin-1-yl]pyrimidin-4-
yl]amino]ethyl]acetamide 552873-05-9P,
N-[2-[[2-(4-Chlorophenyl)-6-[4-[(1,2,3,4-tetrahydronaphthalen-2-
yl)carbonyl]piperazin-1-yl]pyrimidin-4-yl]amino]ethyl]acetamide
R1: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(A2b antagonist; preparation of N-(pyrimidinyl)acetamides as A2b
adenosine
receptor selective antagonists for treatment of asthma, diabetes,
tumors, and other A2b associated diseases)

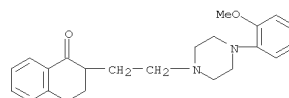
RN 552871-19-9 CAPLUS
CN Acetamide, N-[2-[[2-phenyl-6-[4-[(1,2,3,4-tetrahydro-2-
naphthalenyl)carbonyl]-1-piperazinyl]-4-pyrimidinyl]amino]ethyl]- (CA
INDEX NAME)



RN 552873-05-9 CAPLUS
CN Acetamide, N-[2-[[2-(4-chlorophenyl)-6-[4-[(1,2,3,4-tetrahydro-2-
naphthalenyl)carbonyl]-1-piperazinyl]-4-pyrimidinyl]amino]ethyl]- (CA
INDEX NAME)

L25 ANSWER 32 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2003;362816 Document No. 139;301686 In vivo and in vitro pharmacological
studies of a new hypotensive compound (QF0301B) in rat: Comparison with
prazosin, a known α_1 -adrenoceptor antagonist. Orallo, Francisco;
Garcia-Ferreiro, Tomas; Enguix, Maria Jose; Tristano, Helena; Masaguer,
Cristian; Ravina, Enrique; Cadavid, Isabel; Lora, Maria Isabel
(Department
of Pharmacology, Faculty of Pharmacy, University of Santiago de
Compostela, Santiago de Compostela, 15782, Spain). Vascular
Pharmacology,
40(2), 97-108 (English) 2003. CODEN: VPAHAJ. ISSN: 1537-1891.
Publisher: Elsevier Science Inc..
AB In this work, the authors studied the in vivo and in vitro pharmacol.
effects of the novel compound QF0301B
(2-[2-(N-(4-o-methoxyphenyl)-N-1-piperazinyl)ethyl]-1-tetralone) and
compared with those of prazosin. In anesthetized normotensive rats, both
QF0301B and prazosin (0.1-0.2 mg/kg i.v.) caused a pronounced and
prolonged fall in mean arterial blood pressure accompanied by
bradycardia.
Neither QF0301B nor prazosin (0.2 mg/kg iv) significantly modified the
cardiovascular effects of either 5-hydroxytryptamine (serotonin, 5-HT, 75
 μ g/kg i.v.) or the selective α_2 -adrenoceptor agonist B-HT 920
(0.2 mg/kg i.v.), but both markedly inhibited the hypertensive effect of
noradrenaline (5 μ g/kg i.v.), a nonselective α -adrenergic
receptor agonist. In isolated rubbed rat aorta rings, QF0301B and
prazosin showed marked α_1 -adrenoceptor blocking activity, with pA2
values of 9.00 \pm 0.12 and 9.75 \pm 0.14, resp. In addition, QF0301B reversed
and competitively antagonized the inhibitory action produced by clonidine
in elec. stimulated rat vas deferens and inhibited the force and rate of
contraction in rat isolated atria (pA2=5.91 \pm 0.43), competitively
antagonized the contractile effect of 5-HT in rat aorta (pA2=6.75 \pm 0.06)
and in rat stomach fundus (pA2=7.13 \pm 0.48) and the contractions induced
by histamine in isolated guinea pig longitudinal ileal muscle
(pA2=7.40 \pm 0.40). QF0301B showed noncompetitive low action in 5-HT3,
muscarinic, and nicotinic receptors, or as Ca2+ antagonist. These
results
indicate that a α_1 -adrenoceptor blocking lead was obtained with a
new chemical structure and interesting pharmacol. properties, which only
 α_1 -adrenoceptor blocking activity seems to be responsible for its
cardiovascular effects.

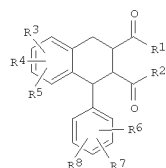
IT 149247-12-1
R1: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU
(Therapeutic use); BIOL (Biological study); USES (Uses)
(new hypotensive compound QF0301B in comparison with prazosin in rats)
RN 149247-12-1 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[2-[[4-(2-methoxyphenyl)-1-
piperazinyl]ethyl]- (CA INDEX NAME)



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L25 ANSWER 33 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2003:173387 Document No. 138:2213680 Preparation of aryl
 tetrahydronaphthalene derivatives as inhibitors of
 P-glycoprotein-mediated
 transport. Melikian-Badalian, Anita (Avlan Limited, UK). PCT Int. Appl.
 WO 2003017948 A2 20030306, 48 pp. DESIGNATED STATES: W: AE, AG, AL, AM,
 AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK,
 DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,
 KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW,
 MX, MY, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM,
 TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ,
 CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC,
 ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2.
 APPLICATION: WO 2002-US27932 20020828. PRIORITY: US 2001-31580P
 20010829.

GI



AB A new family of compds., particularly aryl 1,2,3,4-tetrahydronaphthalene
 derivs. of Formula I [R1, R2 = alkoxy, heterocyclyl, etc.; R3-R8 = H,
 alkyl, alkoxy, Ph, OPh, benzyl, cycloalkyl, etc.], are prepared The
 compds.

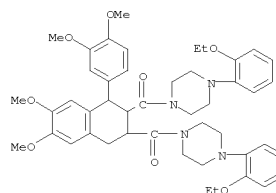
may be used as inhibitors of P-glycoprotein-mediated transport. Use of
 the compds. to enhance bioavailability and to modulate multi-drug
 resistance to chemotherapeutic agents is disclosed.

IT 500614-55-1P 500614-56-2P 500614-57-3P
 500614-64-2P 500614-65-3P 500614-66-4P
 500614-67-5P 500614-74-4P 500614-75-5P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of aryl tetrahydronaphthalene derivs. as inhibitors of
 P-glycoprotein-mediated transport)

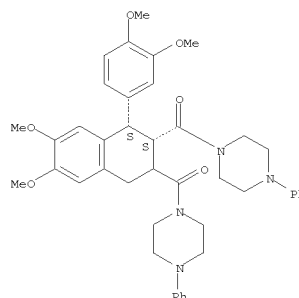
RN 500614-55-1 CAPLUS
 CN Piperazine, 1,1'-[[1-(3,4-dimethoxyphenyl)-1,2,3,4-tetrahydro-6,7-
 dimethoxy-2,3-naphthalenediyl]dicarbonyl]bis[4-(2-ethoxyphenyl)- (9CI)
 (CA INDEX NAME)

L25 ANSWER 33 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 500614-56-2 CAPLUS
 CN Piperazine,
 1,1'-[[1-(1R,2R)-1-(3,4-dimethoxyphenyl)-1,2,3,4-tetrahydro-6,7-
 dimethoxy-2,3-naphthalenediyl]dicarbonyl]bis[4-phenyl-, rel- (9CI) (CA
 INDEX NAME)

Relative stereochemistry.

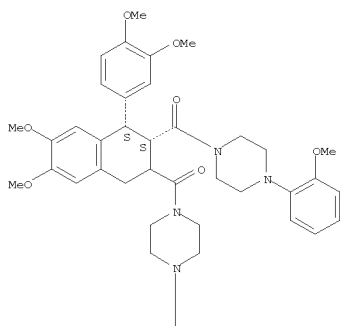


RN 500614-57-3 CAPLUS
 CN Piperazine,
 1,1'-[[1-(1R,2R)-1-(3,4-dimethoxyphenyl)-1,2,3,4-tetrahydro-6,7-
 dimethoxy-2,3-naphthalenediyl]dicarbonyl]bis[4-(2-methoxyphenyl)-, rel-
 (9CI) (CA INDEX NAME)

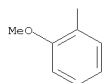
Relative stereochemistry.

L25 ANSWER 33 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

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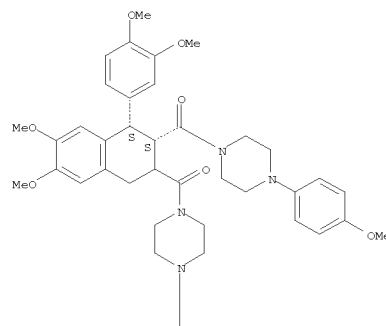


RN 500614-64-2 CAPLUS
 CN Piperazine,
 1,1'-[[1-(1R,2R)-1-(3,4-dimethoxyphenyl)-1,2,3,4-tetrahydro-6,7-
 dimethoxy-2,3-naphthalenediyl]dicarbonyl]bis[4-(4-methoxyphenyl)-, rel-
 (9CI) (CA INDEX NAME)

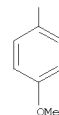
Relative stereochemistry.

L25 ANSWER 33 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

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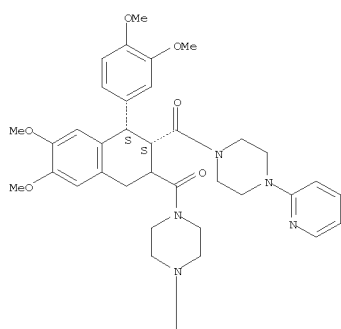
RN 500614-65-3 CAPLUS
 CN Piperazine,
 1,1'-[[1-(1R,2R)-1-(3,4-dimethoxyphenyl)-1,2,3,4-tetrahydro-6,7-
 dimethoxy-2,3-naphthalenediyl]dicarbonyl]bis[4-(2-pyridinyl)-, rel-
 (9CI) (CA INDEX NAME)

Relative stereochemistry.

10590585.trn

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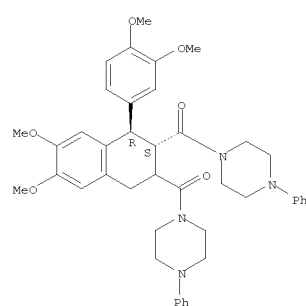
PAGE 2-A



RN 500614-66-4 CAPLUS
CN Piperazine,
1,1'-[[(1R,2S)-1-(3,4-dimethoxyphenyl)-1,2,3,4-tetrahydro-6,7-
dimethoxy-2,3-naphthalenediyl]dicarbonyl]bis[4-phenyl-, rel- (9CI) (CA
INDEX NAME)

Relative stereochemistry.

L25 ANSWER 33 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

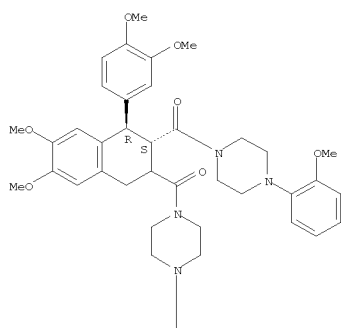


RN 500614-67-5 CAPLUS
CN Piperazine,
1,1'-[[(1R,2S)-1-(3,4-dimethoxyphenyl)-1,2,3,4-tetrahydro-6,7-
dimethoxy-2,3-naphthalenediyl]dicarbonyl]bis[4-(2-methoxyphenyl)-, rel-
(9CI) (CA INDEX NAME)

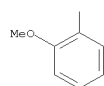
Relative stereochemistry.

L25 ANSWER 33 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

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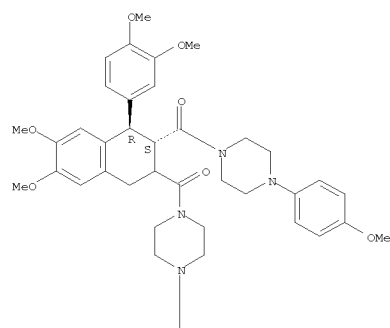


RN 500614-74-4 CAPLUS
CN Piperazine,
1,1'-[[(1R,2S)-1-(3,4-dimethoxyphenyl)-1,2,3,4-tetrahydro-6,7-
dimethoxy-2,3-naphthalenediyl]dicarbonyl]bis[4-(4-methoxyphenyl)-, rel-
(9CI) (CA INDEX NAME)

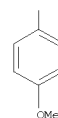
Relative stereochemistry.

L25 ANSWER 33 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

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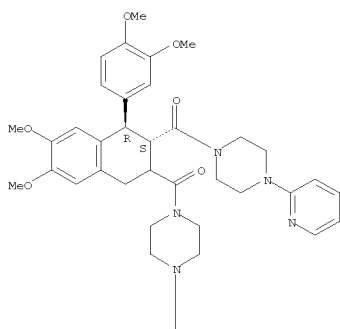
RN 500614-75-5 CAPLUS
CN Piperazine,
1,1'-[[(1R,2S)-1-(3,4-dimethoxyphenyl)-1,2,3,4-tetrahydro-6,7-
dimethoxy-2,3-naphthalenediyl]dicarbonyl]bis[4-(2-pyridinyl)-, rel-
(9CI) (CA INDEX NAME)

Relative stereochemistry.

10590585.trn

L25 ANSWER 33 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

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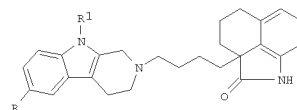


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L25 ANSWER 34 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2002:335088 Document No. 137:631500

2a-[4-(Tetrahydropyridoindol-2-yl)butyl]tetrahydrobenzindole Derivatives: New Selective Antagonists of the 5-Hydroxytryptamine₇ Receptor. Kikuchi, Chika; Ando, Takashi; Watanabe, Takashi; Nagaso, Hiroshi; Okuno, Masayo; Hiranuma, Toyokazu; Koyama, Masao (Pharmaceutical Research Center, Meiji Seika Kaisha Ltd., Kohoku-ku, Yokohama, 222-8567, Japan). Journal of Medicinal Chemistry, 45(11), 2197-2206 (English) 2002. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 137:63150. Publisher: American Chemical Society.

GI



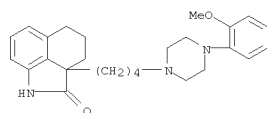
AB Tetrahydrobenzindoles were prepared and their affinity for the 5-hydroxytryptamine₇ (5-HT₇) receptor and other receptors was evaluated. Most of the compds. showed high affinity for the 5-HT₇ receptor, and the [(tetrahydropyridoindolyl)butyl]tetrahydrobenzindoles I (R = H, MeO; R1 = H, Me, MeOCH₂, Ac, allyl, Me₂NCO, H₂NCOCH₂, Me₂NCOCH₂, MeNHCOCH₂) exhibited high selectivity for this receptor. The nature of the substituent at C-9 of the tetrahydropyridoindole ring affected the affinity for the 5-HT₇ receptor and the C-9 carbamoyl substituent afforded increased selectivity. I (R = H; R1 = MeNHCOCH₂) exhibited high affinity for the 5-HT₇ receptor, with at least 280-fold selectivity over the 5-HT₂ receptor. In a functional model of 5-HT₇ receptor activation, this compound was confirmed to have 5-HT₇ receptor antagonist activity. It should be a useful tool for clarifying the biol. role of the 5-HT₇ receptor.

IT 201608-39-1P 201608-45-9P 201608-47-1P
201608-49-3P 201608-51-7P 201608-53-9P
201608-57-3P 201608-69-7P 201608-78-8P
201608-79-9P 201608-91-5P 201608-95-9P
201609-01-0P 201609-20-3P 201609-21-4P
439815-19-7P 439815-21-1P 439815-23-3P
439815-31-3P

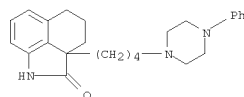
RI: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of piperazinyl-, phenylpiperidinyl-, tetrahydropyridinyl-, and tetrahydropyridoindolylbutylbenzindoles with 5-hydroxytryptamine receptor antagonist activity)

RN 201608-39-1 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)

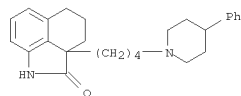
L25 ANSWER 34 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



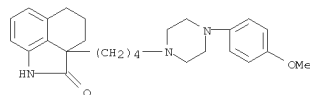
RN 201608-45-9 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-phenyl-1-piperazinyl)butyl]- (CA INDEX NAME)



RN 201608-47-1 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-phenyl-1-piperidinyl)butyl]- (CA INDEX NAME)

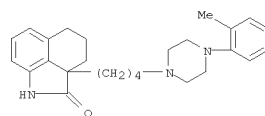


RN 201608-49-3 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(4-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)

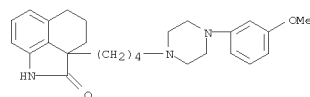


RN 201608-51-7 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-methylphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)

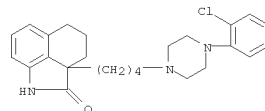
L25 ANSWER 34 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



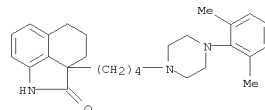
RN 201608-53-9 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(3-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



RN 201608-57-3 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a-[4-[4-(2-chlorophenyl)-1-piperazinyl]butyl]-2a,3,4,5-tetrahydro- (CA INDEX NAME)



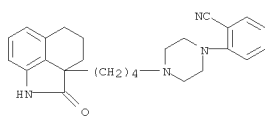
RN 201608-69-7 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a-[4-[4-(2,6-dimethylphenyl)-1-piperazinyl]butyl]-2a,3,4,5-tetrahydro- (CA INDEX NAME)



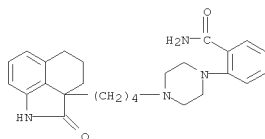
RN 201608-78-8 CAPLUS
CN Benzonitrile, 2-[4-[4-(1,2,4,5-tetrahydro-2-oxobenz[cd]indol-2a(3H)-yl)butyl]-1-piperazinyl]- (CA INDEX NAME)

10590585.trn

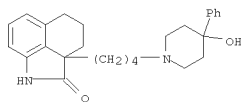
L25 ANSWER 34 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 201608-79-9 CAPLUS
 CN Benzanide,
 2-[4-[4-(1,2,4,5-tetrahydro-2-oxobenz[cd]indol-2a(3H)-yl)butyl]-
 1-piperazinyl]- (CA INDEX NAME)

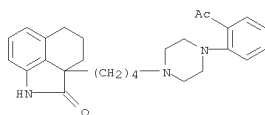


RN 201608-91-5 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-hydroxy-4-phenyl-1-
 piperidinyl)butyl]- (CA INDEX NAME)

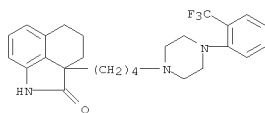


RN 201608-95-9 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-methoxy-4-phenyl-1-
 piperidinyl)butyl]- (CA INDEX NAME)

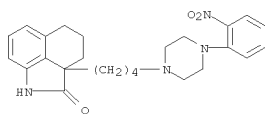
L25 ANSWER 34 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



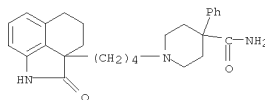
RN 439815-21-1 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-
 (trifluoromethyl)phenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



RN 439815-23-3 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-nitrophenyl)-1-
 piperazinyl]butyl]- (CA INDEX NAME)

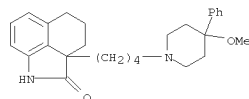


RN 439815-31-3 CAPLUS
 CN 4-Piperidinecarboxamide, 4-phenyl-1-[4-(1,2,4,5-tetrahydro-2-
 oxobenz[cd]indol-2a(3H)-yl)butyl]- (CA INDEX NAME)

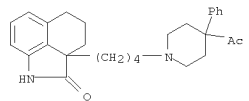


IT 201608-44-8P 201608-46-0P 201608-68-6P
 201608-77-7P 201608-80-2P 201608-94-8P
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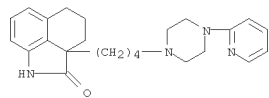
L25 ANSWER 34 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



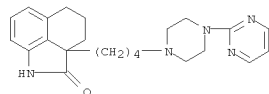
RN 201609-01-0 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a-[4-(4-acetyl-4-phenyl-1-piperidinyl)butyl]-
 2a,3,4,5-tetrahydro- (CA INDEX NAME)



RN 201609-20-3 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-pyridinyl)-1-
 piperazinyl]butyl]- (CA INDEX NAME)



RN 201609-21-4 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-pyrimidinyl)-1-
 piperazinyl]butyl]- (CA INDEX NAME)

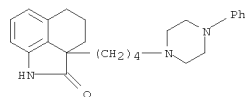


RN 439815-19-7 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a-[4-[4-(2-acetylphenyl)-1-piperazinyl]butyl]-
 2a,3,4,5-tetrahydro- (CA INDEX NAME)

L25 ANSWER 34 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

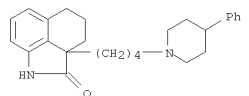
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 439815-24-4P 439815-25-5P 439815-27-7P
 439815-28-8P 439815-30-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of piperazinyl-, phenylpiperidinyl-, tetrahydropyridinyl-, and
 tetrahydropyridoindolylbutylbenzindoles with 5-hydroxytryptamine
 receptor antagonist activity)

RN 201608-44-8 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-phenyl-1-
 piperazinyl)butyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 201608-46-0 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-phenyl-1-
 piperidinyl)butyl]-, hydrochloride (1:1) (CA INDEX NAME)

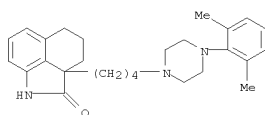


● HCl

RN 201608-68-6 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a-[4-[4-(2,6-dimethylphenyl)-1-
 piperazinyl]butyl]-2a,3,4,5-tetrahydro-, hydrochloride (1:1) (CA INDEX
 NAME)

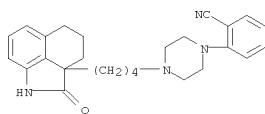
10590585.trn

L25 ANSWER 34 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



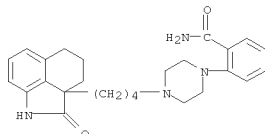
● HCl

RN 201608-77-7 CAPLUS
CN Benzonitrile, 2-[4-[(1,2,4,5-tetrahydro-2-oxobenz[cd]indol-2a(3H)-yl)butyl]-1-piperazinyl]-, hydrochloride (1:1) (CA INDEX NAME)



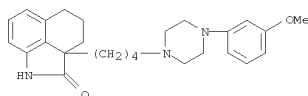
● HCl

RN 201608-80-2 CAPLUS
CN Benzamide, 2-[4-[(1,2,4,5-tetrahydro-2-oxobenz[cd]indol-2a(3H)-yl)butyl]-1-piperazinyl]-, hydrochloride (1:1) (CA INDEX NAME)



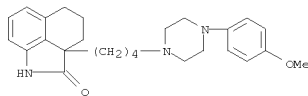
● HCl

L25 ANSWER 34 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



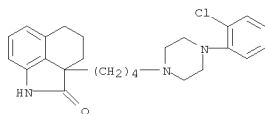
●2 HCl

RN 439815-16-4 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(4-methoxyphenyl)-1-piperazinyl]butyl]-, hydrochloride (1:2) (CA INDEX NAME)



●2 HCl

RN 439815-17-5 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a-[4-[4-(2-chlorophenyl)-1-piperazinyl]butyl]-2a,3,4,5-tetrahydro-, hydrochloride (1:2) (CA INDEX NAME)

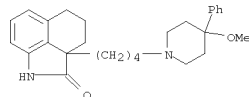


●2 HCl

RN 439815-20-0 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a-[4-[4-(2-acetylphenyl)-1-piperazinyl]butyl]-2a,3,4,5-tetrahydro-, hydrochloride (1:2) (CA INDEX NAME)

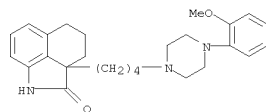
L25 ANSWER 34 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

RN 201608-94-8 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-methoxy-4-phenyl-1-piperidinyl)butyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

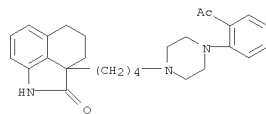
RN 439815-14-2 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-, hydrochloride (1:2) (CA INDEX NAME)



●2 HCl

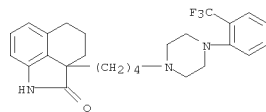
RN 439815-15-3 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(3-methoxyphenyl)-1-piperazinyl]butyl]-, hydrochloride (1:2) (CA INDEX NAME)

L25 ANSWER 34 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



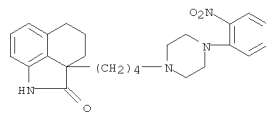
●2 HCl

RN 439815-22-2 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-[2-(trifluoromethyl)phenyl]-1-piperazinyl]butyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 439815-24-4 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-nitrophenyl)-1-piperazinyl]butyl]-, hydrochloride (1:1) (CA INDEX NAME)

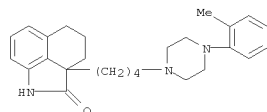


● HCl

RN 439815-25-5 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-methylphenyl)-1-piperazinyl]butyl]-, hydrochloride (1:2) (CA INDEX NAME)

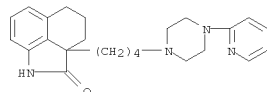
10590585.trn

L25 ANSWER 34 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



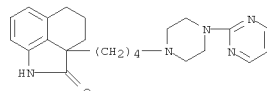
● 2 HCl

RN 439815-27-7 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-pyridinyl)-1-piperazinyl]butyl]-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

RN 439815-28-8 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-pyrimidinyl)-1-piperazinyl]butyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 439815-30-2 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-hydroxy-4-phenyl-1-piperidinyl)butyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 35 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN

2001:886939 Document No. 136:1608570 New Serotonin 5-HT2A, 5-HT2B, and 5-HT2C Receptor Antagonists: Synthesis, Pharmacology, 3D-QSAR, and Molecular Modeling of (Aminoalkyl)benzo and Heterocycloalkanones. Brea, Jose; Rodrigo, Jordi; Carrieri, Antonio; Sanz, Ferran; Cadavid, M. Isabel;

Enquix, Maria J.; Villazon, Maria; Mengod, Guadalupe; Caro, Yolanda; Masquer, Christian F.; Ravina, Enrique; Centeno, Nuria B.; Carotti, Angelo; Loza, M. Isabel (Departamento de Farmacologia Facultad de Farmacia, Universidad de Santiago de Compostela, Santiago de Compostela, E-15782, Spain). Journal of Medicinal Chemistry, 45(1), 54-71 (English) 2002. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 136:160857. Publisher: American Chemical Society.

AB A series of 52 conformationally constrained butyrophenones have been synthesized and pharmacol. tested as antagonists at 5-HT2A, 5-HT2B, and 5-HT2C serotonin receptors, useful for dissecting the role of each 5-HT2 subtype in pathophysiol. These compds. were also a consistent set for

the identification of structural features relevant to receptor recognition and subtype discrimination. Six compds. were found highly active (pKi >

8.76) and selective at the 5-HT2A receptor vs. 5-HT2B and/or 5-HT2C receptors. Piperidine fragments confer high affinity at the 5-HT2A receptor subtype, with benzofuranone- and thiotetralonepiperidine as the most selective derivs. over 5-HT2C and 5-HT2B receptors, resp.; Ki 2A/2C and/or KB 2A/2B ratios greater than 100 were obtained. Compds. showing a more pronounced selectivity at 5-HT2A/5-HT2C than at 5-HT2A/5-HT2B bear 6-fluorobenzisoxazolyl- and p-fluorobenzoylpiperidine moieties

containing one methylene bridging the basic piperidine to the alkanone moiety. An ethylene bridge between the alkanone and the amino moieties led to ligands

with higher affinities for the 5-HT2B receptor. Significant selectivity at the 5-HT2B receptor vs. 5-HT2C was observed with 1-[1-(1-oxo-1,2,3,4-tetrahydro-3-naphthyl)methyl]-4-[3-(p-fluorobenzoyl)propyl]piperazine (more than 100-fold higher). Although piperidine fragments also confer higher affinity at 5-HT2C receptors,

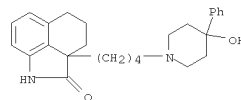
only piperazine-containing ligands were selective over 5-HT2A. Moderate selectivity was observed at 5-HT2C vs. 5-HT2B (10-fold) with some compds. bearing a 4-[3-(6-fluorobenzisoxazolyl)]piperidine moiety in its structure. Mol. determinants for antagonists acting at 5-HT2A receptors were identified by 3D-QSAR (GRID-GOLPE) studies. Docking simulations at 5-HT2A and 5-HT2C receptors suggest a binding site for the studied type

of antagonists (between transmembrane helices 2, 3, and 7) different to that of the natural agonist serotonin (between 3, 5, and 6).

IT 133496-60-3 149247-12-1
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (preparation, QSAR and mol. modeling of (aminoalkyl)benzo and heterocycloalkanones as serotonin 5-HT2A, 5-HT2B, and 5-HT2C receptor antagonists)

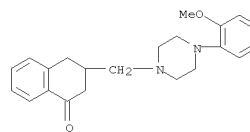
RN 133496-60-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)

L25 ANSWER 34 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

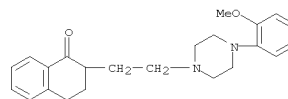


● HCl

L25 ANSWER 35 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 149247-12-1 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[2-[4-(2-methoxyphenyl)-1-piperazinyl]ethyl]- (CA INDEX NAME)



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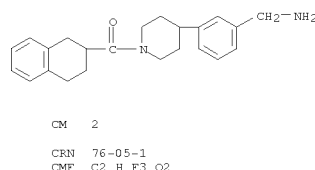
L25 ANSWER 36 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2001:868447 Document No. 136:59170 Preparation of
(hetero)arylacyl-piperidinyl-benzylamines for use as tryptase inhibitors.
Astles, Peter C.; Eastwood, Paul R.; Houille, Olivier; Levell, Julian;
Pauls, Heinz; Czekaj, Mark; Liang, Guyan; Gong, Yong; Pribish, James;
Neuenschwander, Kent (Aventis Pharmaceuticals Products Inc., USA). PCT
Int. Appl. WO 2001090101 A1 20011129, 267 pp. DESIGNATED STATES: W: AE,
AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ,
DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,
JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MW, MN,
MM, MX, ME, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR,
TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ,
TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA,
GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR.
(English). CODEN: PIXXD2. APPLICATION: WO 2001-US13811 20010427.
PRIORITY: GB 2000-12362 20000522; US 2001-843126 20010426.

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

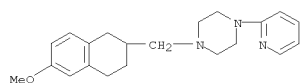
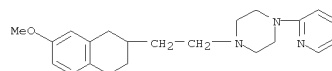
AB Title compds. I [Ar = (hetero)aryl, where the two groups on the Ar ring
are β to each other; R1-2 = H, alkyl; R3 =
(un)substituted(hetero)aryl, arylalkenyl, cycloalkenyl, cycloalkyl, etc.;
R4 = H, acyl, alkoxy, alkylcarbonyl, carboxy, CN, halo, etc.; n = 0 -
4] were prepared Over 300 synthetic examples were disclosed. For
instance,
3-bromobenzylbromide was converted in two steps to boronate II. II was
coupled to the triflate ester derivative of the enol of
4-oxo-N-benzylloxycarbonylpiperidine (DMF, K2CO3, PdCl2(dppf)•CH2Cl2,
80°C, 18 h) to give the corresponding bicyclic intermediate. This
intermediate was deprotected and reduced to the piperidine (EtOH, 10%
Pd-C/H2, room temperature, 5 h) and coupled to
5-phenethylthiophene-2-carboxylic
acid (DMF, HAPyU, iPr2NET, room temperature, 18 h) to give III. III had
Ki = 50
nM for tryptase. I are useful in the treatment of e.g., asthma and
inflammatory diseases.
IT 375852-09-8P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
study); PREP (Preparation); USES (Uses)
(drug; preparation of (hetero)arylacyl-piperidinyl-benzylamines for
use as
tryptase inhibitors)
RN 375852-09-8 CAPLUS
CN Methanone,
[4-[3-(aminomethyl)phenyl]-1-piperidinyl](1,2,3,4-tetrahydro-2-
naphthalenyl)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)
CM 1
CRN 375852-08-7
CMF C23 H28 N2 O

L25 ANSWER 36 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



L25 ANSWER 37 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2001:809680 Document No. 136:857980
trans-4-[4-(4-methoxyphenyl)cyclohexyl]-1-arylpiperazines: A New Class of
Potent and Selective 5-HT1A Receptor Ligands as Conformationally
Constrained Analogues of 4-[3-(5-methoxy-1,2,3,4-tetrahydronaphthalen-1-
yl)propyl]-1-arylpiperazines. Perrone, Roberto; Berardi, Francesco;
Colabufio, Nicola A.; Leopoldo, Marcello; Lacivita, Enza; Tortorella,
Vincenzo; Leonardi, Amedeo; Poggesi, Elena; Testa, Rodolfo (Dipartimento
Farmaco-Chimico, Bari, 70126, Italy). Journal of Medicinal Chemistry,
44(25), 4431-4442 (English) 2001. CODEN: JMCMAR. ISSN: 0022-2623.
OTHER
SOURCES: CASREACT 136:85798. Publisher: American Chemical Society.
AB The influence of conformational parameters on the recognition by rat
5-HT1A receptors of derivs. of 4-[3-(5-methoxy-1,2,3,4-
tetrahydronaphthalen-1-yl)propyl]-1-(2-pyridinyl)piperazine (I) and
3-(5-methoxy-1,2,3,4-tetrahydronaphthalen-1-yl)-N-[2-(2-
pyridyloxy)ethyl]propanamine (II), two highly potent and selective 5-HT1A
receptor ligands, is addressed. Fifteen flexible and rigid analogs were
prepared following several synthetic routes and were tested in binding
assays with radioligands at 5-HT1A, D2, and α 1 receptors from rat
brain membranes. Among the new derivs.
trans-4-[4-[3-(methoxyphenyl)cyclohexyl]-1-(2-pyridinyl)piperazine (III)
and trans-N-[4-[3-(methoxyphenyl)cyclohexyl]-2-(2-pyridyloxy)ethylamine
(IV) emerged as active compds. These compds. can be considered as
conformationally constrained analogs of I and II, resp. In fact, III and
IV showed a marked enhancement in 5-HT1A receptor affinity when compared
to their cis isomers. Because III was a potent and selective 5-HT1A
ligand (Ki, nM: 5-HT1A = 0.028, D2 = 2194, α 1 = 767), it was chosen
as a lead to prepare other analogs that were tested at 5-HT1A, D2, and
 α 1 receptors from rat brain membranes, showing high affinity at the
5-HT1A and selectivity vs D2 and α 1 receptors. Selected compds.
were tested for their affinity at the human cloned 5-HT1A, α 1a,
 α 1b, α 1d receptor subtypes. They were also submitted to the
[35S]GTP γ S binding assay stimulating the 5-HT1A receptor-mediated
G-protein activation, therefore behaving as full or as partial agonists.
Finally, the ability of iv administration of III to induce fore-paw
treading in rats was evaluated in comparison with 8-OH-DPAT. Although
the affinity (Ki) and in vitro activity (pD'2) of III at the 5-HT1A receptor
were higher than those of 8-OH-DPAT, the compound was less potent than
the reference standard in inducing the symptom.
IT 385811-17-6P 385811-22-3P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);
BIOL (Biological study); PREP (Preparation)
(trans-4-[4-(methoxyphenyl)cyclohexyl]-1-arylpiperazines as potent and
selective 5-HT1A receptor agonists)
RN 385811-17-6 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[(1,2,3,4-tetrahydro-6-methoxy-2-
naphthalenyl)methyl]- (CA INDEX NAME)

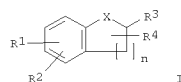
L25 ANSWER 37 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
RN 385811-22-3 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[2-(1,2,3,4-tetrahydro-7-methoxy-2-
naphthalenyl)ethyl]- (CA INDEX NAME)



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L25 ANSWER 38 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2001:521906 Document No. 135:1072590 Lactam derivatives as antiarrhythmic agents. Atwal, Karnail S.; Ahmad, Saleem; Ferrara, Francis N. (Bristol-Myers Squibb Co., USA). U.S. US 6262068 B1 20010717, 17 pp., Cont.-in-part of U.S. Ser. No. 8,948, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1999-231678 19990114. PRIORITY: US 1997-PV38895 19970221; US 1998-8948 19980120.

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AB Lactam derivs. I [X is C(O)NR3'; R1 = halo, alkyl, cycloalkyl, alkyl(cycloalkyl), aryl, (aryl)alkyl, (aryl)alkenyl, (aryl)alkynyl, O-alkyl, O-alkenyl, O-aryl, O-alkyl(aryl), O-alkyl(heterocyclo), etc.; R2

= H, alkyl, halo, aryl, (aryl)alkyl, O-alkyl, amino, substituted amino; R3 and R3' are the same or different and are independently selected from H, alkyl or alkyl(aryl); R4 which can be bonded to a ring carbon or nitrogen,

is selected from hydrogen, alkyl, alkenyl, alkyl(aryl), alkyl(heterocyclo), cycloalkyl, alkyl(cycloalkyl), alkyl(amino), etc.; n is an integer of 0 to

2], useful in the treatment of arrhythmia (no data), were prepared.

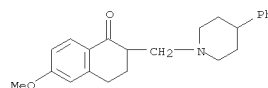
E.g., a multistep synthesis of 3,4-dihydro-6-methoxy-2-[2-(4-phenyl-1-piperidinyl)ethyl]-1(2H)-isoquinolinone monohydrochloride is described. The starting compound for the synthesis was 3,4-dihydro-6-methoxy-1(2H)-isoquinolinone.

IT 212256-36-5P 212256-47-8P 212257-79-9P
 212257-80-2P

RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

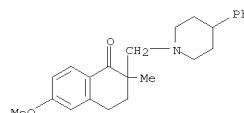
RN 212256-36-5 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 38 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● HCl

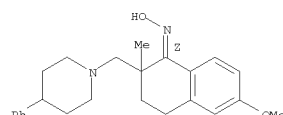
RN 212256-47-8 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-methyl-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 212257-79-9 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-methyl-2-[(4-phenyl-1-piperidinyl)methyl]-, oxime, (1Z)- (CA INDEX NAME)

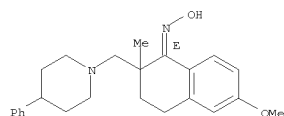
Double bond geometry as shown.



RN 212257-80-2 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-methyl-2-[(4-phenyl-1-piperidinyl)methyl]-, oxime, (1E)- (CA INDEX NAME)

Double bond geometry as shown.

L25 ANSWER 38 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



L25 ANSWER 39 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2001:29942 Document No. 134:231507 N-aryl- or N-alkylpiperazine derivatives:

the role of N-substituent on α_1 , α_2 , 5-HT1A and D2 receptor affinity. Perrone, Roberto; Berardi, Francesco; Colabufo, Nicola A.; Leopoldo, Marcello; Abate, Carmen; Tortorella, Vincenzo (Dipartimento Farmaco-Chimico, Bari, 70126, Italy). Medicinal Chemistry Research, 10(4), 201-207 (English) 2000. CODEN: MCREEB. ISSN: 1054-2523. Publisher: Birkhaeuser Boston.

AB The binding profile at α_1 , α_2 , 5-HT1A and D2 receptors of eight N-substituted-N'-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]piperazines is reported. Results indicated that a suitable substitution can lead to potent 5-HT1A or α_1 , or α_2 ligands.

IT 154744-86-2 330568-39-3

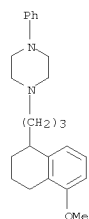
RI: BAC (Biological activity or effector, except adverse); BPR

(Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(role of N-substituent of N-aryl- or N-alkylpiperazine derivs. on α_1 , α_2 , 5-HT1A and D2 receptor affinity)

RN 154744-86-2 CAPLUS

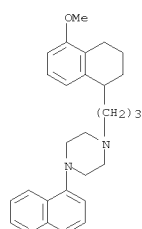
CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)



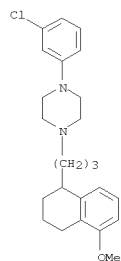
RN 330568-39-3 CAPLUS
 CN Piperazine, 1-(1-naphthalenyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)

10590585.trn

L25 ANSWER 39 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

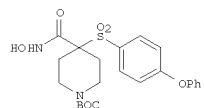


IT 330568-38-2P
 RL: BAC (Biological activity or effector, except adverse); BPR
 (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process) (role of N-substituent of N-aryl- or N-alkylpiperazine derivs. on ol, o2, 5-HT1A and D2 receptor affinity)
 RN 330568-38-2 CAPLUS
 CN Piperazine, 1-(3-chlorophenyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)



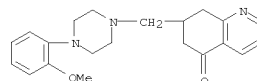
L25 ANSWER 41 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2000:608722 Document No. 133:1930790 Preparation of arylsulfonylheterocyclylhydroxamic acids and related compounds as matrix metalloprotease inhibitors. Barta, Thomas E.; Becker, Daniel P.; Bedell, Louis J.; Boehm, Terri L.; Carroll, Jeffery N.; De Crescenzo, Gary A.; Fobian, Yvette M.; Freskos, John N.; Getman, Daniel P.; McDonald, Joseph J.; Hanson, Gunnar J.; Hockerman, Susan L.; Howard, Susan C.; Kolodziej, Steve A.; Li, Hui; Mischke, Deborah A.; Rico, Joseph G.; Stehle, Nathan W.; Tollefson, Michael B.; Vernier, William F.; Villamil, Clara I.; Rao, Shashidhar N. (G.D. Searle and Co., USA). PCT Int. Appl. WO 2000050396 A1 20000831, 851 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US2518 20000222. PRIORITY: US 1999-256948 19990224.

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AB A process for treating conditions associated with pathol. matrix metalloproteinase (MMP) activity comprises administration of compds. having inhibitory activity against >1 of MMP-2, MMP-9, and MMP-13, while exhibiting substantially less inhibition of MMP-1. The compds. are of the form HONHCOCR1R2SO2R3 [R1, R2 = H; R1R2 = atoms to form a 5-8 membered ring containing 1-3 heteroatoms; R3 = (substituted) aryl, heteroaryl]. Thus, 4-PhOC6H4SH was heated in Me2SO to give the disulfide dimer, which in THF was added to a mixture of Et N-tert-butoxycarbonylisonipecotate (preparation given) and LDA in THF at -60° to room temperature to give 40% sulfide, which was oxidized with m-ClC6H4CO(OOH) to give 59% sulfone. The Et ester was saponified with NaOH in EtOH/H2O to give 100% acid, which in DMF was treated with hydroxybenzotriazole, EDC, 4-methylmorpholine, and aqueous NH2OH to give title compound I. I inhibited MMP-2 with IC50 = 0.2 nM. Pharmacol., pharmacokinetic, and toxicol. data are given for selected compds.
 IT 226393-08-4P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of arylsulfonylheterocyclylhydroxamic acids and related compds.

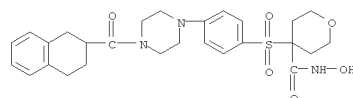
L25 ANSWER 40 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2000:855012 Document No. 134:1629040 A simple, efficient method for regioselective synthesis of 7-aminomethyl-7,8-dihydro-6H-quinolin-5-ones, new potential CNS agents. Pita, B.; Masaguer, C. F.; Ravina, E. (Facultad de Farmacia, Laboratorio de Quimica Farmaceutica, Departamento de Quimica Organica, Universidad de Santiago de Compostela, Santiago de Compostela, 15706, Spain). Tetrahedron Letters, 41(50), 9829-9833 (English) 2000. CODEN: TELEAY. ISSN: 0040-4039. OTHER SOURCES: CASREACT 134:162904. Publisher: Elsevier Science Ltd..
 AB An efficient and convenient strategy for the regioselective synthesis of new conformationally restricted butyrophenones of the quinoline series is presented. 7-(Aminomethyl)-7,8-dihydro-6H-quinolin-5-ones were obtained from 7-(methoxymethyl)-7,8-dihydro-6H-quinolin-5-one via the tosylate, and also in a 1-pot reaction via 7-(bromomethyl)-7,8-dihydro-6H-quinolin-5-one, with moderate-to-good overall yields in both cases.
 IT 325489-07-4P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of (aminomethyl)dihydroquinolinones)
 RN 325489-07-4 CAPLUS
 CN 5(6H)-Quinolinone, 7,8-dihydro-7-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



L25 ANSWER 41 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 as matrix metalloprotease inhibitors)

RN 226393-08-4 CAPLUS
 CN 2H-Pyran-4-carboxamide, tetrahydro-N-hydroxy-4-[[[4-[(1,2,3,4-tetrahydro-2-naphthalenyl)carbonyl]-1-piperazinyl]phenyl]sulfonyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1
 CRN 226393-07-3
 CMF C27 H33 N3 O6 S



CM 2
 CRN 76-05-1
 CMF C2 H F3 O2



10590585.trn

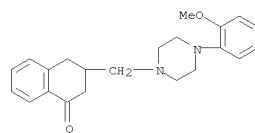
L25 ANSWER 42 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2000;537881 Document No. 133;246811 GRID-Independent Descriptors (GRIND): A Novel Class of Alignment-Independent Three-Dimensional Molecular Descriptors. Pastor, Manuel; Cruciani, Gabriele; McLay, Iain; Pickett, Stephen; Clementi, Sergio (Laboratory on Chemometrics Department of Chemistry, University of Perugia, Perugia, 06123, Italy). Journal of Medicinal Chemistry, 43(17), 3233-3243 (English) 2000. CODEN: JMCMAR. ISSN: 0022-2623. Publisher: American Chemical Society.

AB Traditional methods for performing 3D-QSAR rely upon an alignment step that is often time-consuming and can introduce user bias, the resultant model being dependent upon and sensitive to the alignment used. There are several methods which overcome this problem, but in general the necessary transformations prevent a simple interpretation of the resultant models in the original descriptor space (i.e. 3D mol. coordinates). Here we present a novel class of mol. descriptors which we have termed Grid-Independent Descriptors (GRIND). They are derived in such a way as to be highly relevant for describing biol. properties of compds. while being alignment-independent, chemical interpretable, and easy to compute. GRIND are obtained starting from a set of mol. interaction fields, computed by the program GRID or by other programs. The procedure for computing the descriptors involves a first step, in which the fields are simplified, and a second step, in which the results are encoded into alignment-independent variables using a particular type of autocorrelation transform. The mol. descriptors so obtained can be used to obtain graphical diagrams called "correlograms" and can be used in different chemometric analyses, such as principal component anal. or partial least-squares. An important feature of GRIND is that, with the use of appropriate software, the original descriptors (mol. interaction fields) can be regenerated from the autocorrelation transform and, thus, the results of the anal. represented graphically, together with the original mol. structures, in 3D plots. In this respect, the article introduces the program ALMOND, a software package developed in our group for the computation, anal., and interpretation of GRIND. The use of the methodol. is illustrated using some examples from the field of 3D-QSAR. Highly predictive and interpretable models are obtained showing the promising potential of the novel descriptors in drug design.

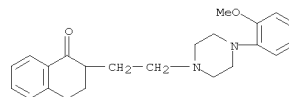
IT 133496-60-3 149247-12-1
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (Grid-Independent Descriptors (GRIND): novel class of alignment-independent three-dimensional mol. descriptors)

RN 133496-60-3 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)

L25 ANSWER 42 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 149247-12-1 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[2-[4-(2-methoxyphenyl)-1-piperazinyl]ethyl]- (CA INDEX NAME)



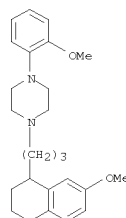
L25 ANSWER 43 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 2000;395917 Document No. 133;202604
 1-Substituted-4-[3-(1,2,3,4-tetrahydro-5- or 7-methoxynaphthalen-1-yl)propyl]piperazines: influence of the N-1 piperazine substituent on 5-HT1A receptor affinity and selectivity versus D2 and α1 receptors. Part 6. Perrone, R.; Berardi, F.; Colabufo, N. A.; Leopoldo, M.; Tortorella, V. (Dipartimento Farmaco-Chimico, Universita degli Studi di Bari, Bari, 70126, Italy). Bioorganic & Medicinal Chemistry, 8(5), 873-881 (English) 2000. CODEN: BMECEP. ISSN: 0968-0896. Publisher: Elsevier Science Ltd..

AB In the present paper, we report the synthesis and the binding profiles on 5-HT1A, D2, and α1 receptors of 1-substituted-4-[3-(5- or 7-methoxy-1,2,3,4-tetrahydronaphthalen-1-yl)propyl]piperazine derivs. and some related heteroalkyl derivs. The results obtained are compared to those previously reported for the 1-Ph, 1-(2-methoxyphenyl), 1-(2-pyridyl) analogs. The results pointed out the critical role of the group linked in the N-1 position of the piperazine in terms of 5-HT1A binding affinity. In fact, 1-cyclohexyl, 1-(3-benzisoxazolyl), 1-(benzothiazole-2-carbonyl), 1-(2-benzothiazolyl), 1-(2-quinolyl) substituted piperazines displayed moderate or low 5-HT1A receptor affinity; on the contrary, 1-(3-benzisothiazolyl) and 1-(1-naphthalenyl) substituted piperazines displayed high 5-HT1A receptor affinity, the KI values being in the subnanomolar range. Furthermore, three compds. demonstrated better selectivity over α1 receptors than the reference compds.

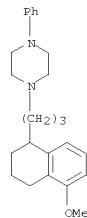
IT 154744-84-OP 154744-86-2P 154744-87-3P
 154744-88-4P 154744-89-5P 184346-64-3P
 290370-34-2P 290370-35-3P 290370-37-5P
 290370-38-6P
 RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
 (substituent on 5-HT1A receptor affinity and selectivity vs. D2 and α1 receptors of arylpiperazine deriv)

RN 154744-84-0 CAPLUS
 CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)

L25 ANSWER 43 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



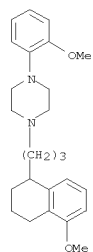
RN 154744-86-2 CAPLUS
 CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)



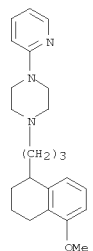
RN 154744-87-3 CAPLUS
 CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)

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L25 ANSWER 43 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

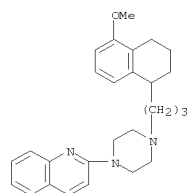


RN 154744-88-4 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)



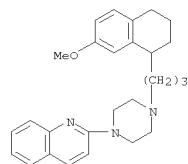
RN 154744-89-5 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)

L25 ANSWER 43 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● 2 HCl

RN 290370-35-3 CAPLUS
CN Quinoline,
2-[4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]-1-piperazinyl]-, hydrochloride, hydrate (1:2:1) (CA INDEX NAME)

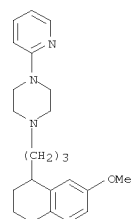


● 2 HCl

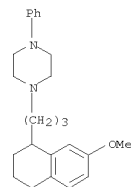
● H₂O

RN 290370-37-5 CAPLUS
CN Piperazine, 1-(1-naphthalenyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 43 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

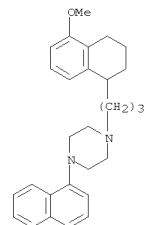


RN 184346-64-3 CAPLUS
CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)



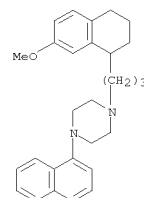
RN 290370-34-2 CAPLUS
CN Quinoline,
2-[4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]-1-piperazinyl]-, hydrochloride (1:2) (CA INDEX NAME)

L25 ANSWER 43 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● HCl

RN 290370-38-6 CAPLUS
CN Piperazine, 1-(1-naphthalenyl)-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

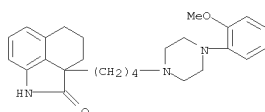
10590585.trn

L25 ANSWER 44 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2000:379675 Document No. 133:159635 First pharmacophoric hypothesis for 5-HT7 antagonism. Lopez-Rodriguez, Maria L.; Porraz, Esther; Benhamu, Bellinda; Ramos, Jose A.; Morcillo, M. Jose; Lavandera, Jose L. (Departamento de Quimica Organica I, Facultad de Ciencias Quimicas, Universidad Complutense, Madrid, E-28040, Spain). Bioorganic & Medicinal Chemistry Letters, 10(10), 1097-1100 (English) 2000. CODEN: BMCLE8. ISSN: 0960-894X. Publisher: Elsevier Science Ltd..

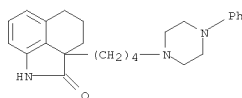
AB In order to make the first contribution to the elucidation of essential structural features for 5-HT7 antagonism, a set of 30 5-HT7 antagonists were selected from the literature. A pharmacophore model was built using mol. modeling studies with Catalyst program. The information contained

in this model was validated with newly synthesized compds.
IT 201608-39-1 201608-45-9 201608-78-8
201608-87-9 201608-88-0 201609-20-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study) (pharmacophoric hypothesis for 5-HT7 antagonism)

RN 201608-39-1 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



RN 201608-45-9 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-phenyl-1-piperazinyl)butyl]- (CA INDEX NAME)

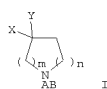


RN 201608-78-8 CAPLUS
CN Benzonitrile, 2-[4-[4-(1,2,4,5-tetrahydro-2-oxobenz[cd]indol-2a(3H)-yl)butyl]-1-piperazinyl]- (CA INDEX NAME)

L25 ANSWER 45 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2000:335384 Document No. 132:3474900 Preparation of piperidines as ORL-1 receptor ligands.. Barlocco, Daniela; Cignarella, Giorgio; Giardina, Giuseppe Arnaldo Maria; Grugni, Mario; Ronzoni, Silvano (Smithkline Beecham Spa, Italy). PCT Int. Appl. WO 2000/27815 A2 20000518, 75 pp. DESIGNATED STATES: W: CA, JP, US; RW: AT, BE, CH, CY, DE, DK, ES, FI,

FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1999-EP8706 19991110. PRIORITY: IT 1998-MI2442 19981111.

GI

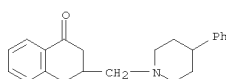


AB Title compds. [I; X, Y = H, (substituted) aryl; m, n = 0-3, provided that m and n are not both 0; A = bond, (C(R1)R2)P; P = 1-3; R1, R2 = H, halo, (substituted) alkyl, alkoxy; B = C4-8 (unsatd.) (substituted) ring], were prepared. Thus, 2,3-dihydro-2-[(4-phenylpiperidin-1-yl)carbonyl]-1H-indene was stirred with LiAlH4 in THF to give 2,3-dihydro-2-[(4-phenylpiperidin-1-yl)methyl]-1H-indene. The most potent

I showed ORL-1 binding with Ki = 1-1000 nM.
IT 69797-43-9P 109132-90-3P 126684-43-3P
269084-27-7P 269084-28-8P 269084-29-9P
269084-30-2P 269084-87-9P 269084-88-0P
269084-89-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of piperidines as ORL-1 receptor ligands)

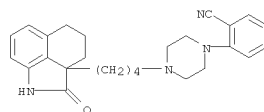
RN 69797-43-9 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



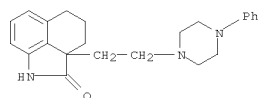
● HCl

RN 109132-90-3 CAPLUS
CN Piperidine, 4-phenyl-1-[(1,2,3,4-tetrahydro-2-naphthalenyl)methyl]- (CA INDEX NAME)

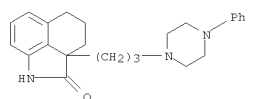
L25 ANSWER 44 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



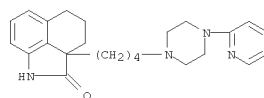
RN 201608-87-9 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[2-(4-phenyl-1-piperazinyl)ethyl]- (CA INDEX NAME)



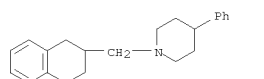
RN 201608-88-0 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[3-(4-phenyl-1-piperazinyl)propyl]- (CA INDEX NAME)



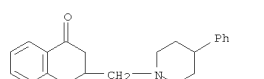
RN 201609-20-3 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-(2-pyridinyl)-1-piperazinyl)butyl]- (CA INDEX NAME)



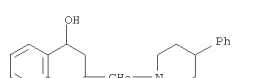
L25 ANSWER 45 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



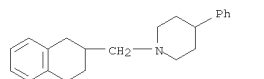
RN 126684-43-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[(4-phenyl-1-piperidinyl)methyl]- (CA INDEX NAME)



RN 269084-27-7 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-3-[(4-phenyl-1-piperidinyl)methyl]- (CA INDEX NAME)



RN 269084-28-8 CAPLUS
CN Piperidine, 4-phenyl-1-[(1,2,3,4-tetrahydro-2-naphthalenyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



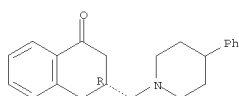
● HCl

RN 269084-29-9 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1), (3R)- (CA INDEX NAME)

Absolute stereochemistry.

10590585.trn

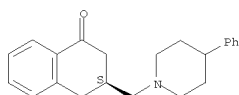
L25 ANSWER 45 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● HCl

RN 269084-30-2 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1), (3S)- (CA INDEX NAME)

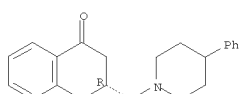
Absolute stereochemistry.



● HCl

RN 269084-87-9 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[(4-phenyl-1-piperidinyl)methyl]-, (3R)- (CA INDEX NAME)

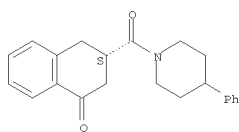
Absolute stereochemistry.



RN 269084-88-0 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[(4-phenyl-1-piperidinyl)methyl]-, (3S)- (CA INDEX NAME)

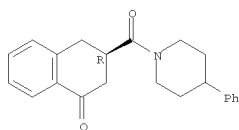
Absolute stereochemistry.

L25 ANSWER 45 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

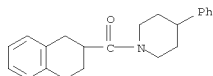


RN 269084-15-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[(4-phenyl-1-piperidinyl)carbonyl]-, (3R)- (CA INDEX NAME)

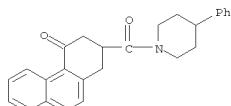
Absolute stereochemistry.



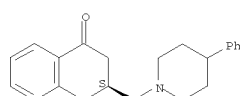
RN 269084-16-4 CAPLUS
CN Methanone, (4-phenyl-1-piperidinyl) (1,2,3,4-tetrahydro-2-naphthalenyl)- (CA INDEX NAME)



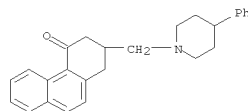
RN 269084-17-5 CAPLUS
CN 4(1H)-Phenanthrenone, 2,3-dihydro-2-[(4-phenyl-1-piperidinyl)carbonyl]- (CA INDEX NAME)



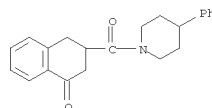
L25 ANSWER 45 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 269084-89-1 CAPLUS
CN 4(1H)-Phenanthrenone, 2,3-dihydro-2-[(4-phenyl-1-piperidinyl)methyl]- (CA INDEX NAME)



IT 269084-13-1P 269084-14-2P 269084-15-3P
269084-16-4P 269084-17-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of piperidines as ORL-1 receptor ligands)
RN 269084-13-1 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[(4-phenyl-1-piperidinyl)carbonyl]- (CA INDEX NAME)

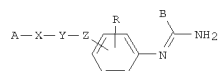


RN 269084-14-2 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[(4-phenyl-1-piperidinyl)carbonyl]-, (3S)- (CA INDEX NAME)

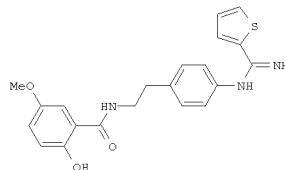
Absolute stereochemistry.

L25 ANSWER 46 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
2000:210150 Document No. 132:2510670 Novel amidine derivatives, their preparation and application as inhibitors of NO synthase and lipid peroxidation, and pharmaceutical compositions containing them. Auvin, Serge; Chabrier de Lazauniere, Pierre-Etienne; Harnett, Jeremiah; Pons, Dominique; Ulibarri, Gerard (Societe de Conseils de Recherches et d'Applications Scientifiques (S.C.R.A.S., Fr.). PCT Int. Appl. WO 2000017190 A2 20000330, 119 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (French). CODEN: PIXXD2. APPLICATION; WO 1999-FR2250 19990922. PRIORITY: FR 1998-11868 19980923.

GI



I

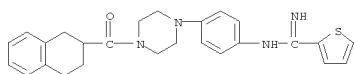


II

AB The invention concerns novel amidine derivs., including compds. I [R = H, alkyl, alkoxy; A = certain substituted aryl or (un)substituted heteroaryl groups; B = alkyl, (un)substituted aryl or heteroaryl, (un)substituted or heterocyclic amino; X = bond, (CH2)m, O(CH2)m, (CH2)mO, S(CH2)m, O(CH2)mCO, CH:CH, etc.; Y = bond, (CH2)n, (CH2)rQ(CH2)s; Q = piperazine, homopiperazine, piperidine, pyrrolidine, azetidine, thiazolidine, saturated C3-7 carbocycles, etc.; Z = bond, (CH2)pO(CH2)q, (CH2)pS(CH2)q, (CH2)pNH(CH2)q, etc.; m, n, p, q, r, s = 0-6, as well as addnl. specific compds. In particular, 2-hydroxy-5-methoxy-N-[2-[4-[(2-thienyliminomethyl)amino]phenyl]ethyl]benzamide (II) and 2,5-dihydroxy-N-[2-[4-[(2-thienyliminomethyl)amino]phenyl]ethyl]benzamide are disclosed. Also disclosed are the use of I as medicines, and pharmaceutical compds. containing them. For instance, amidation of 5-methoxysalicylic acid with 4-nitrophenethylamine-HCl, followed by hydrogenation of the nitro group to amino, condensation of the amine with

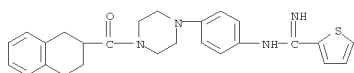
10590585.trn

L25 ANSWER 46 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
S-methyl-2-thiophenethiocarboximide-HI, and acidification in acetone,
gave II.HCl. The IC50 of selected I, including II.HCl, against rat neuronal
NO synthase in vitro, was < 3.5 µM.
IT 262613-20-7P 262614-14-2P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of amidine derivs. as inhibitors of NO
synthase and/or lipid peroxidn.)
RN 262613-20-7 CAPLUS
CN 2-Thiophenecarboximidamide, N-[4-[4-[(1,2,3,4-tetrahydro-2-
naphthalenyl)carbonyl]-1-piperazinyl]phenyl]-, hydrochloride (1:1) (CA
INDEX NAME)



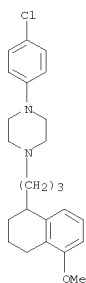
● HCl

RN 262614-14-2 CAPLUS
CN 2-Thiophenecarboximidamide, N-[4-[4-[(1,2,3,4-tetrahydro-2-
naphthalenyl)carbonyl]-1-piperazinyl]phenyl]- (CA INDEX NAME)

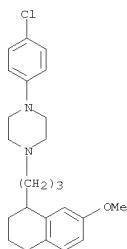


L25 ANSWER 47 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1999;815373 Document No. 132:165762 A structure-affinity relationship study
on derivatives of N-[2-[4-(4-chlorophenyl)piperazin-1-yl]ethyl]-3-
methoxybenzamide, a high-affinity and selective D4 receptor ligand.
Perrone, Roberto; Berardi, Francesco; Colabufio, Nicola A.; Leopoldo,
Marcello; Tortorella, Vincenzo (Dipartimento Farmaco-Chimico, Universita
di Bari, Bari, 70126, Italy). Journal of Medicinal Chemistry, 43(2),
270-277 (English) 2000. CODEN: JMCMAR. ISSN: 0022-2623. Publisher:
American Chemical Society.
AB N-[2-[4-(4-Chlorophenyl)piperazin-1-yl]ethyl]-3-methoxybenzamide, a
high-affinity and selective dopamine D4 receptor ligand, was chosen as a
lead, and structural modifications were done on its amide bond and on its
alkyl chain linking the benzamide moiety to the piperazine ring and by
preparing some semirigid analogs. The binding profile at dopamine D4 and
dopamine D2, serotonin 5-HT1A, and adrenergic α1 receptors of 16 new
comps. was determined From the results emerged that the modification
of the amide bond and the elongation of the intermediate alkyl chain caused a
decrease in dopamine D4 receptor affinity. All prepared semirigid
analog displayed D4 receptor affinity values in the same range of the opened
counterparts.
IT 258882-67-6P 258882-68-7P 258882-79-0P
258882-80-3P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
study, unclassified); SPN (Synthetic preparation); BIOL (Biological
study); PREP (Preparation)
(preparation of derivs. of
[[chlorophenyl]piperazinyl]ethyl]methoxybenzamid
e as selective D4 receptor ligand)
RN 258882-67-6 CAPLUS
CN Piperazine, 1-(4-chlorophenyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-
naphthalenyl)propyl]- (CA INDEX NAME)

L25 ANSWER 47 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

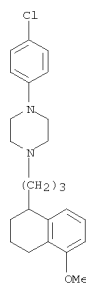


RN 258882-68-7 CAPLUS
CN Piperazine, 1-(4-chlorophenyl)-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-
naphthalenyl)propyl]- (CA INDEX NAME)



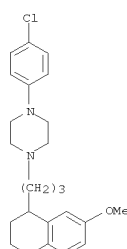
RN 258882-79-0 CAPLUS
CN Piperazine, 1-(4-chlorophenyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-
naphthalenyl)propyl]-, hydrochloride (1:2) (CA INDEX NAME)

L25 ANSWER 47 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● 2 HCl

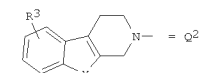
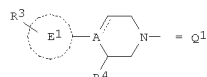
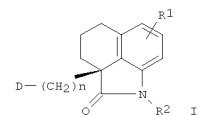
RN 258882-80-3 CAPLUS
CN Piperazine, 1-(4-chlorophenyl)-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-
naphthalenyl)propyl]-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

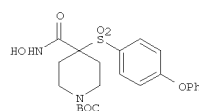
10590585.trn

L25 ANSWER 48 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1999:691080 Document No. 131:2994660 Preparation of optically active tetrahydrobenzindole derivatives having affinity to 5-HT7 receptor. Koyama, Masao; Ushiroda, Osamu; Kikuchi, Chika; Ando, Takashi; Sato, Eriko; Okuno, Masayo; Hiranuma, Toyokazu (Meiji Seika Kaisha, Ltd., Japan). PCT Int. Appl. WO 9954303 A1 19991028, 56 pp. DESIGNATED STATES:
 W: CA, CN, JP, KR, NO, US; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (Japanese). CODEN: PIXXD2.
 APPLICATION:
 WO 1999-JP2127 19990421. PRIORITY: JP 1998-111833 19980422.
 GI



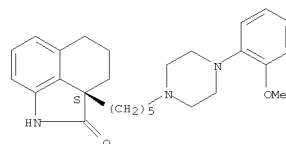
AB Title compds. I (R1, R3 = H, halo, alkyl, etc.; R2, R4 = H, alkyl, aralkyl; n = 2, 3, 4; D = Q1, Q2, etc; E1 = a group forming a benzene ring, etc.; A = N, CH, etc.; X = O, S, etc.; dotted line = optional double bond) and their pharmaceutically acceptable salts, useful in the treatment or prevention of mental diseases, are prepared. Thus, reaction of (S)-2a-(4-bromobutyl)-2a,3,4,5-tetrahydro-1H-benz[cd]indol-2-one with 1,2,3,4-tetrahydroisoquinoline in DMF in the presence of K2CO3 gave 100% (S)-2a-[4-(1,2,3,4-tetrahydroisoquinolin-2-yl)butyl]-2a,3,4,5-tetrahydro-1H-benz[cd]indol-2-one (II). In tests for affinity for 5-HT7 receptor, II had a Ki value of 7.7 nM.
 IT 247082-14-0P

L25 ANSWER 49 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1999:350651 Document No. 131:189290 Preparation of arylsulfonyletheterocyclylhydroxamic acids and related compounds as matrix metalloprotease inhibitors. Barta, Thomas E.; Becker, Daniel P.; Boehm, Terri L.; De Crescenzo, Gary A.; Villamil, Clara I.; McDonald, Joseph J.; Freskos, John N.; Getman, Daniel P. (G.D. Searle and Co., USA). PCT Int. Appl. WO 9925687 A1 19990527, 840 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GD, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US23242 19981112. PRIORITY: US 1997-66007 19971114.
 GI

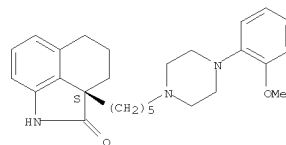


AB A process for treating conditions associated with pathol. matrix metalloproteinase (MMP) activity comprises administration of compds. having inhibitory activity against >1 of MMP-2, MMP-9, and MMP-13, while exhibiting substantially less inhibition of MMP-1. The compds. are of the form HONHCOCR1R2SO2R3 [R1, R2 = H; R1R2 = atoms to form a 5-8 membered ring containing 1-3 heteroatoms; R3 = (substituted) aryl, heteroaryl]. Thus, 4-PhOC6H4SH was heated in Me2SO to give the disulfide dimer, which in THF was added to a mixture of Et N-tert-butoxycarbonylisoleucinate (preparation given) and LDA in THF at -60° to room temperature to give 40% sulfide, which was oxidized with m-ClC6H4CO(OOH) to give 59% sulfone. The Et ester was saponified with NaOH in EtOH/H2O to give 100% acid, which in DMF was treated with hydroxybenzotriazole, EDC, 4-methylmorpholine, and aqueous NH2OH to give title compound (I). I inhibited MMP-2 with IC50 = 0.2 nM.
 IT 226393-08-4P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of arylsulfonyletheterocyclylhydroxamic acids and related compds. as matrix metalloprotease inhibitors)
 RN 226393-08-4 CAPLUS
 CN 2H-Pyran-4-carboxamide, tetrahydro-N-hydroxy-4-[[4-[(1,2,3,4-tetrahydro-2-naphthalenyl)carbonyl]-1-piperazinyl]phenyl]sulfonyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

L25 ANSWER 48 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of optically active tetrahydrobenzindole derivs. having affinity to 5-HT7 receptor)
 RN 247082-14-0 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[5-[4-(2-methoxyphenyl)-1-piperazinyl]pentyl]-, (2aS)- (CA INDEX NAME)
 Absolute stereochemistry. Rotation (+).

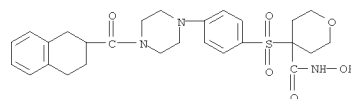


IT 247082-15-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of optically active tetrahydrobenzindole derivs. having affinity to 5-HT7 receptor)
 RN 247082-15-1 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[5-[4-(2-methoxyphenyl)-1-piperazinyl]pentyl]-, hydrochloride (1:1), (2aS)- (CA INDEX NAME)
 Absolute stereochemistry. Rotation (+).



● HCl

L25 ANSWER 49 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 CM 1
 CRN 226393-07-3
 CMF C27 H33 N3 O6 S



CM 2
 CRN 76-05-1
 CMF C2 H F3 O2



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L25 ANSWER 50 OF 96 CAPLUS COPYRIGHT 2010 ACS ON STN
 1999:65930 Document No. 130:276228 Tetrahydrobenzindoles: Selective Antagonists of the 5-HT₇ Receptor. Kikuchi, Chika; Nagaso, Hiroshi; Hiranuma, Toyokazu; Koyama, Masao (Pharmaceutical Research Center, Meiji Seika Kaisha Ltd., Yokohama, 222-8567, Japan). Journal of Medicinal Chemistry, 42(4), 533-535 (English) 1999. CODEN: JMCMAR. ISSN: 0022-2623. Publisher: American Chemical Society.

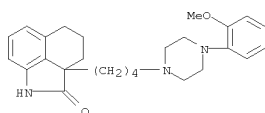
AB A novel series of tetrahydrobenzindoles was synthesized and tested for affinity towards 5-HT₇ and other receptors. Some of the compds. showed high affinity and high selectivity for the 5-HT₇ receptor. 2A-[4-(4-Phenyl-1,2,3,6-tetrahydropyridyl)butyl]-2a,3,4,5-tetrahydrobenzo[cd]indol-2(1H)one (I) was a highly potent ligand for the 5-HT₇ receptor, with at least 47-fold selectivity over the 5-HT₂ receptor and other receptors. A limited structure-activity relationship study for these derivs. indicated that an aromatic ring is required for affinity

for the 5-HT₇ and 5-HT₂ receptors. I was evaluated in a functional model of the 5-HT₇ receptor activation and confirmed to be a 5-HT₇ receptor antagonist.

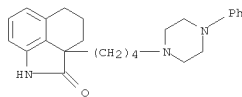
IT 201608-39-1 201608-45-9 201608-78-8
 201608-87-9 201608-88-0 201609-20-3
 RL: BFR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
 (preparation and structure activity of tetrahydrobenzindoles and

towards 5-HT₇ receptor antagonist activity)

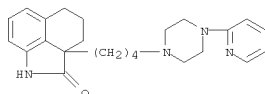
RN 201608-39-1 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



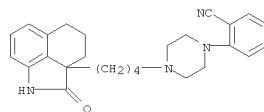
RN 201608-45-9 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-phenyl-1-piperazinyl)butyl]- (CA INDEX NAME)



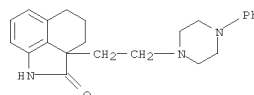
L25 ANSWER 50 OF 96 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)



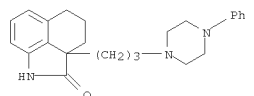
L25 ANSWER 50 OF 96 CAPLUS COPYRIGHT 2010 ACS ON STN (Continued)
 RN 201608-78-8 CAPLUS
 CN Benzonitrile, 2-[4-[4-(1,2,4,5-tetrahydro-2-oxobenz[cd]indol-2a(3H)-yl)butyl]-1-piperazinyl]- (CA INDEX NAME)



RN 201608-87-9 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[2-(4-phenyl-1-piperazinyl)ethyl]- (CA INDEX NAME)



RN 201608-88-0 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[3-(4-phenyl-1-piperazinyl)propyl]- (CA INDEX NAME)



RN 201609-20-3 CAPLUS
 CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-pyridinyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



L25 ANSWER 51 OF 96 CAPLUS COPYRIGHT 2010 ACS ON STN
 1999:59416 Document No. 130:196622
 1-Aryl-4-[(5-methoxy-1,2,3,4-tetrahydronaphthalen-1-yl)alkyl]piperazines and Their Analogs: Influence of the Stereochemistry of the Tetrahydronaphthalen-1-yl Nucleus on 5-HT_{1A} Receptor Affinity and Selectivity versus α_1 and D₂ Receptors. 5. Perrone, Roberto; Berardi, Francesco; Colabufio, Nicola A.; Leopoldo, Marcello; Tortorella, Vincenzo (Dipartimento Farmaco-Chimico, Universita di Bari, Bari, 70126, Italy). Journal of Medicinal Chemistry, 42(3), 490-496 (English) 1999. CODEN: JMCMAR. ISSN: 0022-2623. Publisher: American Chemical Society.

AB Some 1-aryl-4-[(5-methoxy-1,2,3,4-tetrahydronaphthalen-1-yl)propyl]piperazines and their alkylamino and alkylamido analogs, previously studied as 5-HT_{1A} ligands, were prepared in enantiomerically pure form, and their absolute configuration was determined by chemical correlation or by chiroptical properties. They were evaluated for in vitro 5-HT_{1A}, D₂, and α_1 receptor affinity by radioligand binding assays, to study the influence of the chiral carbon atom of the tetrahydronaphthalene nucleus on the 5-HT_{1A} affinity and selectivity. Results indicated that, as regarding the 5-HT_{1A} receptor affinity, there was no difference in affinity between (-)- and (+)-enantiomers as well as the racemate of each compound. The stereochem., instead, influenced the selectivity: all (-)-enantiomers displayed affinity values higher than those of

(+)-isomers at D₂ receptors, and conversely, all (+)-enantiomers displayed affinity values higher than those of (-)-isomers at α_1 receptors. As a result of this trend, it is not possible to predict the isomer with the better selectivity profile. However, (+)-isomers displayed high affinity for the 5-HT_{1A} receptor (IC₅₀ 2,3-7.0 nM) and good selectivity (≥250-fold) vs. both D₂ and α_1 receptors. Furthermore, (S)-(+)- and (R)-(-)-4-[3-(5-methoxy-1,2,3,4-tetrahydronaphthalen-1-yl)propyl]-1-(2-pyridyl)piperazine were submitted to the [35S]GTPγS binding assay for a preliminary evaluation of their intrinsic activity on the 5-HT_{1A} receptor.

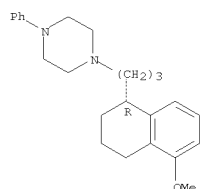
IT 220832-25-7P 220832-26-8P 220832-27-9P
 220832-28-0P 220832-29-1P 220832-30-4P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (aryl[1-methoxytetrahydronaphthyl]alkyl)piperazines and their 5-HT_{1A} receptor affinity and selectivity vs. α_1 and D₂ receptors)

RN 220832-25-7 CAPLUS
 CN Piperazine, 1-phenyl-4-[3-[(1R)-1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl]propyl]-, hydrochloride (1:2) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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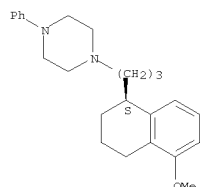
L25 ANSWER 51 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



●2 HCl

RN 220832-26-8 CAPLUS
CN Piperazine, 1-phenyl-4-[3-[(1S)-1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl]propyl]-, hydrochloride (1:2) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



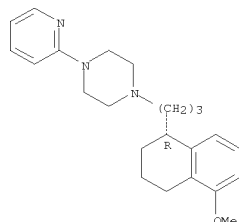
●2 HCl

RN 220832-27-9 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-[(1R)-1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl]propyl]-, hydrochloride (1:2) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L25 ANSWER 51 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

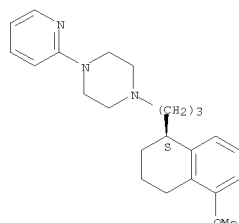
Absolute stereochemistry. Rotation (-).



●2 HCl

RN 220832-30-4 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[3-[(1S)-1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl]propyl]-, hydrochloride (1:2) (CA INDEX NAME)

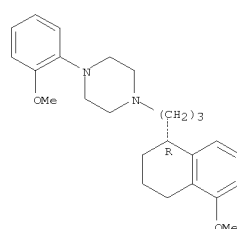
Absolute stereochemistry. Rotation (+).



●2 HCl

IT 220831-82-3P 220831-84-5P 220831-86-7P
220831-88-9P 220831-90-3P 220831-92-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(aryl(methoxytetrahydronaphthyl)alkylpiperazines and their 5-HT1A receptor affinity and selectivity vs. α1 and D2 receptors)

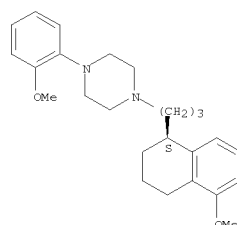
L25 ANSWER 51 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



●2 HCl

RN 220832-28-0 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-[(1S)-1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl]propyl]-, hydrochloride (1:2) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



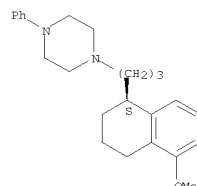
●2 HCl

RN 220832-29-1 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[3-[(1R)-1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl]propyl]-, hydrochloride (1:2) (CA INDEX NAME)

L25 ANSWER 51 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

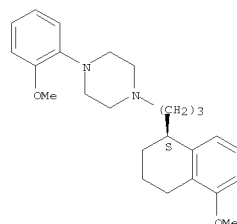
RN 220831-82-3 CAPLUS
CN Piperazine, 1-phenyl-4-[3-[(1S)-1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl]propyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 220831-84-5 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-[(1S)-1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl]propyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

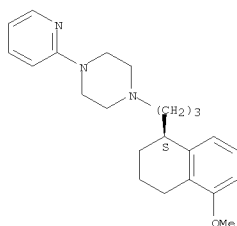


RN 220831-86-7 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[3-[(1S)-1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl]propyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

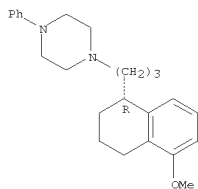
10590585.trn

L25 ANSWER 51 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 220831-88-9 CAPLUS
CN Piperazine, 1-phenyl-4-[3-[(1R)-1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl]propyl]- (CA INDEX NAME)

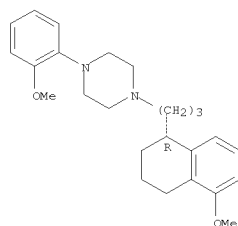
Absolute stereochemistry. Rotation (-).



RN 220831-90-3 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-[(1R)-1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl]propyl]- (CA INDEX NAME)

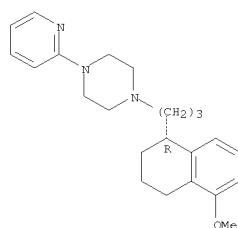
Absolute stereochemistry. Rotation (-).

L25 ANSWER 51 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 220831-92-5 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[3-[(1R)-1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl]propyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L25 ANSWER 52 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1998:703905 Document No. 130:90062

N-[2-[4-(4-Chlorophenyl)piperazin-1-yl]ethyl]-3-methoxybenzamide: A

Potent

and Selective Dopamine D4 Ligand. Perrone, Roberto; Berardi, Francesco; Colabufo, Nicola A.; Leopoldo, Marcello; Tortorella, Vincenzo (Dipartimento Farmaco-Chimico, Universita di Bari, Bari, 70126, Italy). Journal of Medicinal Chemistry, 41(24), 4903-4909 (English) 1998. CODEN: JMCMAR. ISSN: 0022-2623. Publisher: American Chemical Society.

AB A series of new 1-aryl-4-alkylpiperazines containing a terminal benzamide fragment or a tetralin-1-yl nucleus on the alkyl chain were synthesized and tested for binding at cloned human dopamine D4 and D2 receptor subtypes. A SAFIR (structure-affinity relationship) study on this series is herein discussed. The most relevant D4 receptor affinities were displayed by N-[ω-[4-aryl]piperazin-1-yl]alkyl]-methoxybenzamides, their IC50 values ranging between 0.057 and 7.8 nM. Among these, N-[2-[4-(4-chlorophenyl)piperazin-1-yl]ethyl]-3-methoxybenzamide (I) emerged since it exhibited very high affinity for dopamine D4 receptor (IC50 = 0.057 nM) with selectivity of >10 000 for the D4 vs. the D2 receptor; compound I was also selective vs. serotonin 5-HT1A and

adrenergic

α1 receptors.

IT 154744-84-0 154744-87-3

RL: BAC (Biological activity or effector, except adverse); BSU

(Biological

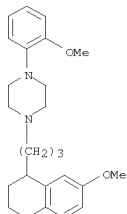
study, unclassified); PRP (Properties); BIOL (Biological study)

(preparation of piperazinyl benzamides as dopamine D4 ligands and potential

antipsychotics)

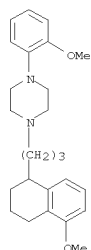
RN 154744-84-0 CAPLUS

CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)



RN 154744-87-3 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)

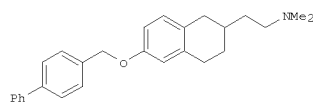
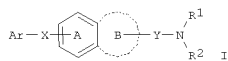
L25 ANSWER 52 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



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L25 ANSWER 53 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1998:608594 Document No. 129:2164280 Original Reference No.
 129:43999a,44002a Preparation of 2-aminoalkyltetralines as amyloid- β
 production inhibitors. Kato, Kaneyoshi; Terauchi, Jun; Fukumoto,
 Hiroaki;
 Kakihana, Mitsuru (Takeda Chemical Industries, Ltd., Japan). PCT Int.
 Appl. WO 9838156 A1 19980903, 238 pp. DESIGNATED STATES: W: AL, AM, AU,
 AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GW, HU, ID, IL, IS, KG,
 KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG,
 SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD,
 RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CL, CM, DE, DK, ES, FI, FR,
 GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG.
 (English). CODEN: PIXXD2. APPLICATION: WO 1998-JP780 19980226.
 PRIORITY: JP 1997-43940 19970227; JP 1997-193497 19970718.

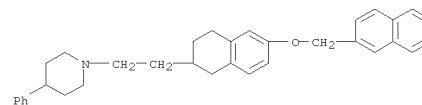
GI



AB The title compds. [I; Ar = (un)substituted aromatic ring, fused aromatic
 group;
 X = a bond, S, SO, SO2, etc.; Y = (un)substituted divalent C1-6 aliphatic
 hydrocarbon group optionally containing O or S; R1, R2 = H, lower alkyl;
 NR1R2
 = (un)substituted N-containing heterocyclic ring; Ring A =
 (un)substituted
 benzene; Ring B = (un)substituted 4-8 membered ring] and their salts,
 which have the effect of inhibiting amyloid- β protein production and/or
 secretion and are useful for preventing and/or treating the
 neurodegenerative disease such as Alzheimer's disease, were prepared and
 formulated. Thus, treatment of [6-(4-biphenyl)methoxy-2-tetralin]-N,N-
 dimethylacetamide with LiAlH4 in THF afforded II.HCl which showed 74% and
 75% inhibition of the production and/or secretion of A β 1-40 and
 A β 1-42, resp.
 IT 212571-19-2P
 RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological

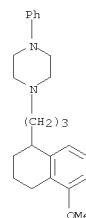
L25 ANSWER 54 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1998:606943 Document No. 129:312907 Original Reference No.
 129:63785a,63788a
 Synthesis and biodistribution of (R,S)-[O-methyl-11C]-1-[3-(5-methoxy-
 1,2,3,4-tetrahydro-1-naphthalenyl)propyl]-4-phenylpiperazine
 (PNU-157760),
 a putative radioligand for 5-HT1A receptors. Matarrese, Mario; Soloviev,
 Dmitriy V.; Moresco, Rosa M.; Ferri, Valentino; Simonelli, Pasquale;
 Magni, Fulvio; Colombo, Diego; Todde, Sergio; Carpinelli, Assunta; Fazio,
 Ferruccio; Kienle, Marzia Galli (CNR INB, Institute H. S. Raffaele,
 University of Milan, Milan, Italy). Bioorganic Chemistry, 26(2), 91-102
 (English) 1998. CODEN: BOCMBM. ISSN: 0045-2068. Publisher: Academic
 Press.
 AB Racemic 1-[3-(5-methoxy-1,2,3,4-tetrahydro-1-naphthalenyl)propyl]-4-
 phenylpiperazine (PNU-157760) was labeled with carbon-11 (t1/2 = 20.4
 min)
 as a putative radioligand for the noninvasive assessment of 5-HT1A
 receptors in vivo with positron emission tomog. (PET). The radiochem.
 synthesis consisted of O-methylation of desmethyl precursor with
 [11C]methyl iodide in the presence of potassium tert-butoxide in DMF. The
 desmethyl precursor for the radiosynthesis of [11C]PNU-157760, was
 prepared
 by a convenient one-step demethylation of PNU-157760 with boron
 tribromide. (R,S)-[O-methyl-11C]-1-[3-(5-methoxy-1,2,3,4-tetrahydro-1-
 naphthalenyl)propyl]-4-phenylpiperazine with >99% radiochem. purity was
 obtained in 30 min with a radiochem. yield of 10 \pm 5% (EOS, nondecay
 corrected) and a specific radioactivity of 2.5 \pm 1 Ci/ μ mol.
 Biodistribution studies in rats showed that [11C]PNU-157760 readily
 crosses the blood-brain barrier with a maximum of brain uptake at 30 min
 after injection; however, the low specific-to-nonspecific binding ratio
 in
 vivo as evidenced by the low hippocampus/cerebellum uptake ratio (1.17 at
 60 min postinjection) does not make [11C]PNU-157760 a promising
 radioligand for serotonin 5-HT1A receptors. (c) 1998 Academic Press.
 IT 214957-40-1P
 RL: BPR (Biological process); BSU (Biological study, unclassified); SPN
 (Synthetic preparation); BIOL (Biological study); PREP (Preparation);
 PROC
 (Process)
 (Synthesis and biodistribution of
 (R,S)-[O-methyl-11C]-1-[3-(5-methoxy-1,2,3,4-tetrahydro-1-
 naphthalenyl)propyl]-4-phenylpiperazine, a putative radioligand for
 5-HT1A receptors)
 RN 214957-40-1 CAPLUS
 CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-5-(methoxy-11C)-1-
 naphthalenyl)propyl]- (9CI) (CA INDEX NAME)

L25 ANSWER 53 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of 2-aminoalkyltetralines as amyloid- β prodrn. inhibitors)
 RN 212571-19-2 CAPLUS
 CN Piperidine,
 4-phenyl-1-[2-[1,2,3,4-tetrahydro-6-(2-naphthalenylmethoxy)-2-
 naphthalenyl]ethyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L25 ANSWER 54 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 Synthesis and biodistribution of (R,S)-[O-methyl-11C]-1-[3-(5-methoxy-
 1,2,3,4-tetrahydro-1-naphthalenyl)propyl]-4-phenylpiperazine
 (PNU-157760),
 a putative radioligand for 5-HT1A receptors. Matarrese, Mario; Soloviev,
 Dmitriy V.; Moresco, Rosa M.; Ferri, Valentino; Simonelli, Pasquale;
 Magni, Fulvio; Colombo, Diego; Todde, Sergio; Carpinelli, Assunta; Fazio,
 Ferruccio; Kienle, Marzia Galli (CNR INB, Institute H. S. Raffaele,
 University of Milan, Milan, Italy). Bioorganic Chemistry, 26(2), 91-102
 (English) 1998. CODEN: BOCMBM. ISSN: 0045-2068. Publisher: Academic
 Press.
 AB Racemic 1-[3-(5-methoxy-1,2,3,4-tetrahydro-1-naphthalenyl)propyl]-4-
 phenylpiperazine (PNU-157760) was labeled with carbon-11 (t1/2 = 20.4
 min)
 as a putative radioligand for the noninvasive assessment of 5-HT1A
 receptors in vivo with positron emission tomog. (PET). The radiochem.
 synthesis consisted of O-methylation of desmethyl precursor with
 [11C]methyl iodide in the presence of potassium tert-butoxide in DMF. The
 desmethyl precursor for the radiosynthesis of [11C]PNU-157760, was
 prepared
 by a convenient one-step demethylation of PNU-157760 with boron
 tribromide. (R,S)-[O-methyl-11C]-1-[3-(5-methoxy-1,2,3,4-tetrahydro-1-
 naphthalenyl)propyl]-4-phenylpiperazine with >99% radiochem. purity was
 obtained in 30 min with a radiochem. yield of 10 \pm 5% (EOS, nondecay
 corrected) and a specific radioactivity of 2.5 \pm 1 Ci/ μ mol.
 Biodistribution studies in rats showed that [11C]PNU-157760 readily
 crosses the blood-brain barrier with a maximum of brain uptake at 30 min
 after injection; however, the low specific-to-nonspecific binding ratio
 in
 vivo as evidenced by the low hippocampus/cerebellum uptake ratio (1.17 at
 60 min postinjection) does not make [11C]PNU-157760 a promising
 radioligand for serotonin 5-HT1A receptors. (c) 1998 Academic Press.
 IT 214957-40-1P
 RL: BPR (Biological process); BSU (Biological study, unclassified); SPN
 (Synthetic preparation); BIOL (Biological study); PREP (Preparation);
 PROC
 (Process)
 (Synthesis and biodistribution of
 (R,S)-[O-methyl-11C]-1-[3-(5-methoxy-1,2,3,4-tetrahydro-1-
 naphthalenyl)propyl]-4-phenylpiperazine, a putative radioligand for
 5-HT1A receptors)
 RN 214957-40-1 CAPLUS
 CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-5-(methoxy-11C)-1-
 naphthalenyl)propyl]-, hydrochloride (1:2) (CA INDEX NAME)

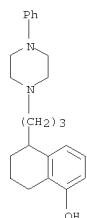


●2 HCl

IT 214957-39-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (synthesis and biodistribution of
 (R,S)-[O-methyl-11C]-1-[3-(5-methoxy-1,2,3,4-tetrahydro-1-
 naphthalenyl)propyl]-4-phenylpiperazine, a putative radioligand for
 5-HT1A receptors)
 RN 214957-39-8 CAPLUS
 CN 1-Naphthalenol, 5,6,7,8-tetrahydro-5-[3-(4-phenyl-1-piperazinyl)propyl]-

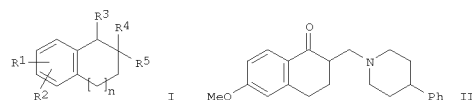
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L25 ANSWER 54 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
(CA INDEX NAME)



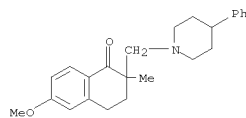
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1998:603193 Document No. 129:2164200 Original Reference No.
129:43995a,43998a Preparation of tetralone derivatives as antiarrhythmic agents. Ahmad, Saleem; Stein, Philip D.; Ferrara, Francis N.; Atwal, Karnail S. (Bristol-Myers Squibb Co., USA). PCT Int. Appl. WO 9836749 A1 19980827, 204 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US2338 19980207.
PRIORITY: US 1997-38917 19970221.

GI



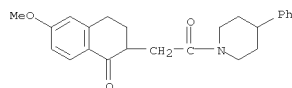
AB The title compds. [I; R1 = halo, alkyl, alkenyl, etc.; R2 = H, alkyl, halo, etc.; R3 = O, OH, alkoxy, etc.; R4 = H, alkyl, alkyl(COalkyl), alkyl(COOalkyl); R3R4 taken together with the atoms to which they are attached form a 5-7 membered ring containing up to three heteroatoms selected from O, N and S; R5 = H, alkyl, alkenyl, etc.; n = 0-2], useful in the treatment of arrhythmia, were prepared. Thus, treatment of 6-methoxytetralone with paraformaldehyde and N-methylanilinium trifluoroacetate in THF followed by reaction of the resulting 2-methylene-6-methoxy-1-tetralone with 4-phenylpiperidine over alumina in PhMe afforded the title compound II. Compds. I are effective at 0.001-10 mg/kg/day.
IT 212256-47-8P 212256-71-8P 212256-91-2P
212257-97-1P 212257-98-2P 212258-02-1P
212258-21-4P 212258-22-5P 212258-76-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of tetralones as antiarrhythmic agents)
RN 212256-47-8 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

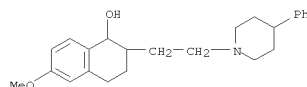


● HCl

RN 212256-71-8 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[2-oxo-2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

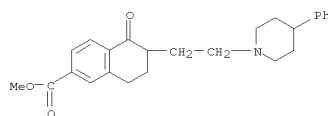


RN 212256-91-2 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-methoxy-2-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)



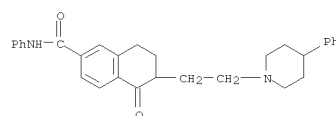
● HCl

RN 212257-97-1 CAPLUS
CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, methyl ester (CA INDEX NAME)

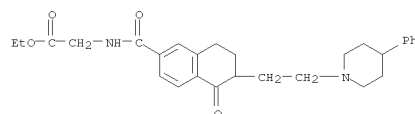


L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

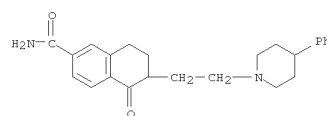
RN 212257-98-2 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-N-phenyl-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212258-02-1 CAPLUS
CN Glycine,
N-[[5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-2-naphthalenyl]carbonyl]-, ethyl ester (CA INDEX NAME)



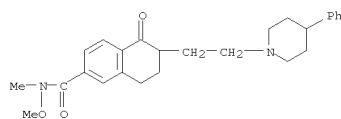
RN 212258-21-4 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



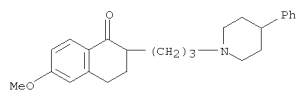
RN 212258-22-5 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-N-methoxy-N-methyl-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

10590585.trn

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

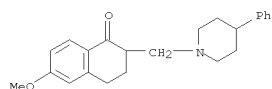


RN 212258-76-9 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[3-(4-phenyl-1-piperidinyl)propyl]- (CA INDEX NAME)



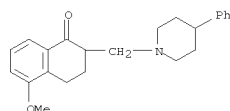
IT 109132-88-9P 212256-36-5P 212256-39-8P
212256-40-1P 212256-42-3P 212256-43-4P
212256-44-5P 212256-45-6P 212256-51-4P
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212257-68-6P 212257-79-9P 212257-80-2P
212257-82-4P 212257-83-5P 212257-84-6P
212257-85-7P 212257-86-8P 212257-88-0P
212257-89-1P 212257-90-4P 212257-91-5P
212257-93-7P 212257-94-8P 212257-95-9P
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212258-05-4P 212258-06-5P 212258-07-6P
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L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



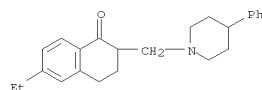
● HCl

RN 212256-39-8 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-5-methoxy-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 212256-40-1 CAPLUS
CN 1(2H)-Naphthalenone, 6-ethyl-3,4-dihydro-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

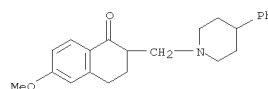
RN 212256-42-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-(phenylmethoxy)-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

212258-11-2P 212258-12-3P 212258-13-4P
212258-14-5P 212258-15-6P 212258-16-7P
212258-17-8P 212258-18-9P 212258-19-0P
212258-20-3P 212258-23-6P 212258-24-7P
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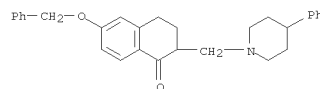
RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of tetralones as antiarrhythmic agents)

RN 109132-88-9 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[(4-phenyl-1-piperidinyl)methyl]- (CA INDEX NAME)



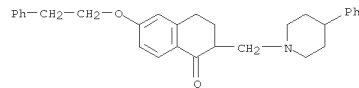
RN 212256-36-5 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



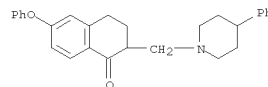
● HCl

RN 212256-43-4 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-(2-phenylethoxy)-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 212256-44-5 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-phenoxy-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

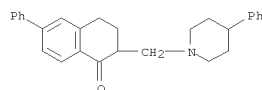


● HCl

RN 212256-45-6 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-phenyl-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

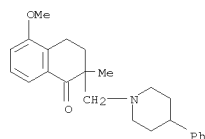
10590585.trn

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



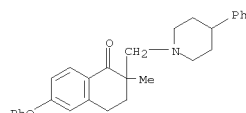
● HCl

RN 212256-51-4 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-5-methoxy-2-methyl-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 212256-52-5 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-methyl-6-phenoxy-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



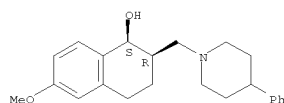
● HCl

RN 212256-53-6 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-methyl-6-phenyl-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

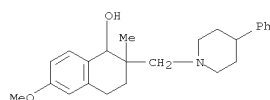
RN 212256-57-0 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-methoxy-2-[(4-phenyl-1-piperidinyl)methyl]-, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.

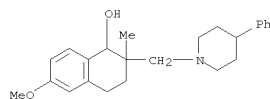


● HCl

RN 212256-58-1 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-methoxy-2-methyl-2-[(4-phenyl-1-piperidinyl)methyl]-, (1R,2S)-rel- (CA INDEX NAME)



RN 212256-59-2 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-methoxy-2-methyl-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

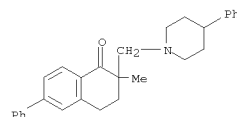


● HCl

RN 212256-63-8 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-(phenylmethoxy)-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

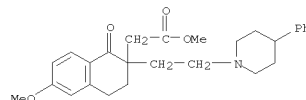
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

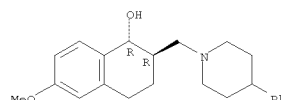
RN 212256-54-7 CAPLUS
CN 2-Naphthaleneacetic acid, 1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-[2-(4-phenyl-1-piperidinyl)ethyl]-, methyl ester, hydrochloride (1:1) (CA INDEX NAME)



● HCl

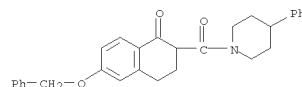
RN 212256-55-8 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-methoxy-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1), (1R,2R)-rel- (CA INDEX NAME)

Relative stereochemistry.

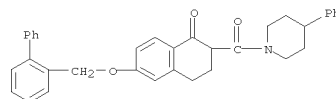


● HCl

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

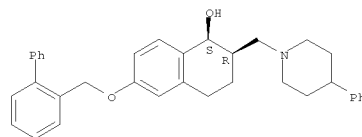


RN 212256-66-1 CAPLUS
CN 1(2H)-Naphthalenone, 6-([1,1'-biphenyl]-2-ylmethoxy)-3,4-dihydro-2-[(4-phenyl-1-piperidinyl)methyl]-, (1R,2S)-rel- (CA INDEX NAME)

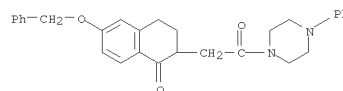


RN 212256-70-7 CAPLUS
CN 1-Naphthalenol, 6-([1,1'-biphenyl]-2-ylmethoxy)-1,2,3,4-tetrahydro-2-[(4-phenyl-1-piperidinyl)methyl]-, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.



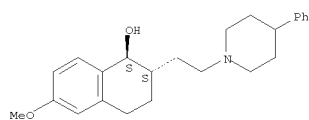
RN 212256-72-9 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[2-oxo-2-(4-phenyl-1-piperazinyl)ethyl]-6-(phenylmethoxy)-, (1R,2R)-rel- (CA INDEX NAME)



RN 212256-92-3 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-methoxy-2-[2-(4-phenyl-1-piperidinyl)ethyl]-, (1R,2R)-rel- (CA INDEX NAME)

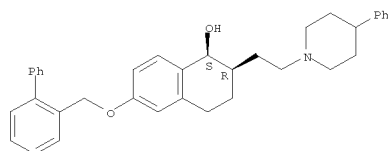
10590585.trn

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
Relative stereochemistry.



RN 212256-93-4 CAPLUS
CN 1-Naphthalenol,
6-([1,1'-biphenyl]-2-ylmethoxy)-1,2,3,4-tetrahydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]-, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.



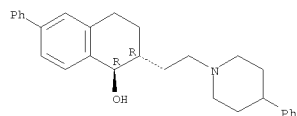
RN 212256-94-5 CAPLUS
CN 1-Naphthalenol,
6-([1,1'-biphenyl]-2-ylmethoxy)-1,2,3,4-tetrahydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]-, (1R,2S)-rel-,
(2R,3R)-2,3-dihydroxybutanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 212256-93-4
CMP C36 H39 N O2

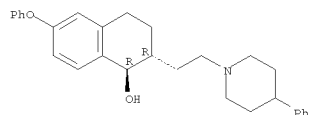
Relative stereochemistry.

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



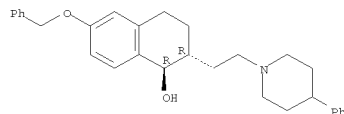
RN 212256-98-9 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-phenoxy-2-[2-(4-phenyl-1-piperidinyl)ethyl]-, (1R,2R)-rel- (CA INDEX NAME)

Relative stereochemistry.



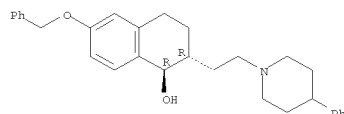
RN 212257-02-8 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-(phenylmethoxy)-2-[2-(4-phenyl-1-piperidinyl)ethyl]-, (1R,2R)-rel-(+)- (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

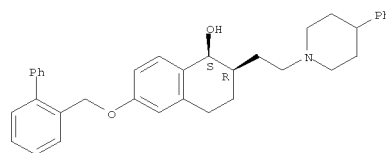


RN 212257-03-9 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-(phenylmethoxy)-2-[2-(4-phenyl-1-piperidinyl)ethyl]-, (1R,2R)-rel-(-)- (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



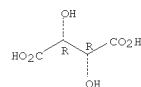
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 2

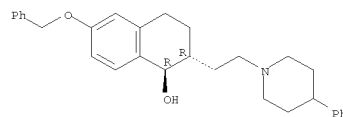
CRN 87-69-4
CMP C4 H6 O6

Absolute stereochemistry.



RN 212256-96-7 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-(phenylmethoxy)-2-[2-(4-phenyl-1-piperidinyl)ethyl]-, (1R,2R)-rel- (CA INDEX NAME)

Relative stereochemistry.

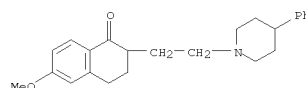


RN 212256-97-8 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-phenyl-2-[2-(4-phenyl-1-piperidinyl)ethyl]-, (1R,2R)-rel- (CA INDEX NAME)

Relative stereochemistry.

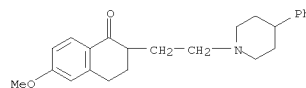
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

RN 212257-24-4 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

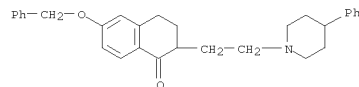


● HCl

RN 212257-25-5 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212257-26-6 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-(phenylmethoxy)-2-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

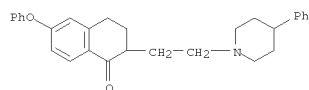


● HCl

RN 212257-27-7 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-phenoxy-2-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

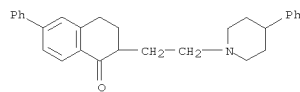
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L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



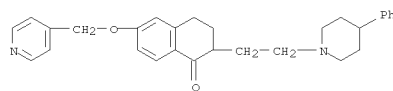
● HCl

RN 212257-28-8 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-phenyl-2-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

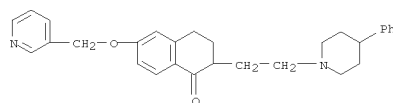
RN 212257-29-9 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]-6-(4-pyridinylmethoxy)-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

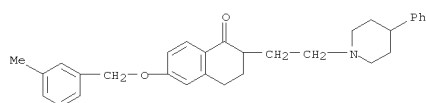
RN 212257-30-2 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-(2-phenylethyl)-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

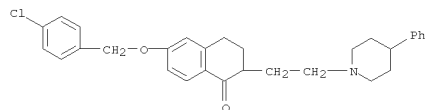


● 2 HCl

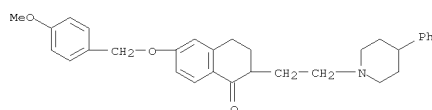
RN 212257-34-6 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-[(3-methylphenyl)methoxy]-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212257-35-7 CAPLUS
CN 1(2H)-Naphthalenone, 6-[(4-chlorophenyl)methoxy]-3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

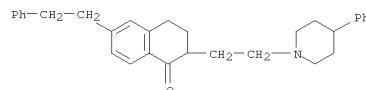


RN 212257-36-8 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-[(4-methoxyphenyl)methoxy]-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

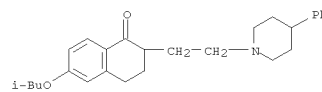


RN 212257-37-9 CAPLUS

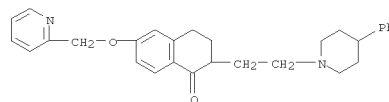
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 212257-31-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-(2-methylpropoxy)-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212257-32-4 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]-6-(2-pyridinylmethoxy)-, hydrochloride (1:2) (CA INDEX NAME)

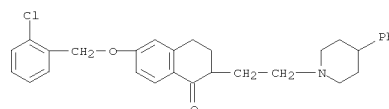


● 2 HCl

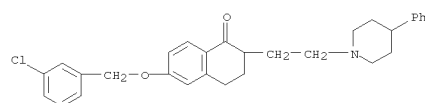
RN 212257-33-5 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]-6-(3-pyridinylmethoxy)-, hydrochloride (1:2) (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

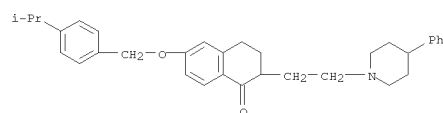
CN 1(2H)-Naphthalenone, 6-[(2-chlorophenyl)methoxy]-3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



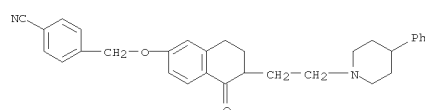
RN 212257-38-0 CAPLUS
CN 1(2H)-Naphthalenone, 6-[(3-chlorophenyl)methoxy]-3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212257-39-1 CAPLUS
CN 1(2H)-Naphthalenone, 4-[[[5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-2-naphthalenyl]oxy]methyl]- (CA INDEX NAME)

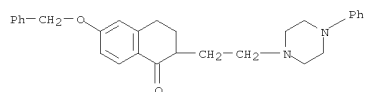


RN 212257-40-4 CAPLUS
CN Benzonitrile, 4-[[[5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-2-naphthalenyl]oxy]methyl]- (CA INDEX NAME)

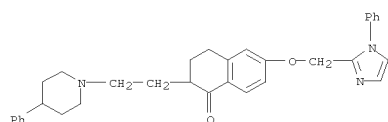


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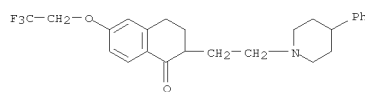
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 RN 212257-44-8 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-(phenylmethoxy)-2-[2-(4-phenyl-1-piperazinyl)ethyl]- (CA INDEX NAME)



RN 212257-47-1 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-[(1-phenyl-1H-imidazol-2-yl)methoxy]-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



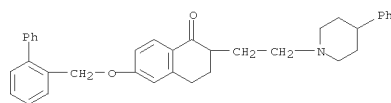
RN 212257-48-2 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]-6-(2,2,2-trifluoroethoxy)-, hydrochloride (1:1) (CA INDEX NAME)



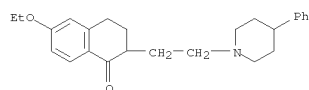
● HCl

RN 212257-49-3 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-[(3-nitrophenyl)methoxy]-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

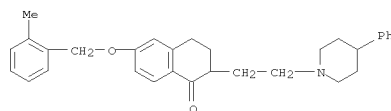
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



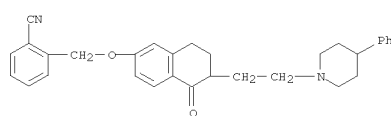
RN 212257-54-0 CAPLUS
 CN 1(2H)-Naphthalenone, 6-ethoxy-3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212257-55-1 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-[(2-methylphenyl)methoxy]-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

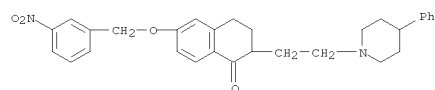


RN 212257-57-3 CAPLUS
 CN Benzonitrile, 2-[[[5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-2-naphthalenyl]oxy]methyl]- (CA INDEX NAME)

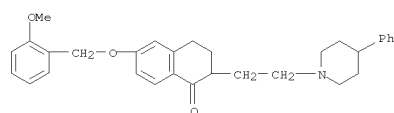


RN 212257-58-4 CAPLUS
 CN Benzoic acid, 4-[[[5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-2-naphthalenyl]oxy]methyl]-, methyl ester (CA INDEX NAME)

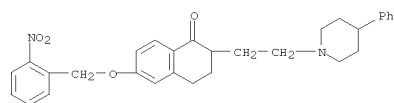
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



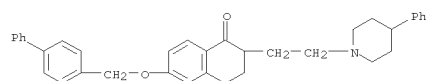
RN 212257-50-6 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-[(2-methoxyphenyl)methoxy]-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212257-51-7 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-[(2-nitrophenyl)methoxy]-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

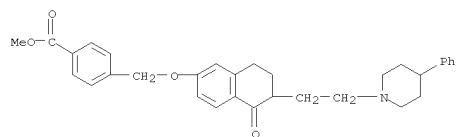


RN 212257-52-8 CAPLUS
 CN 1(2H)-Naphthalenone, 6-[[[1,1'-biphenyl]-4-ylmethoxy]-3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

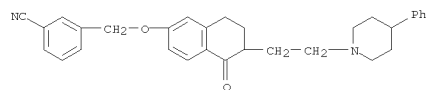


RN 212257-53-9 CAPLUS
 CN 1(2H)-Naphthalenone, 6-[[[1,1'-biphenyl]-2-ylmethoxy]-3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

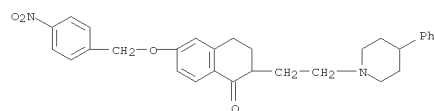
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



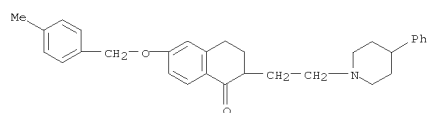
RN 212257-59-5 CAPLUS
 CN Benzonitrile, 3-[[[5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-2-naphthalenyl]oxy]methyl]- (CA INDEX NAME)



RN 212257-60-8 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-[(4-nitrophenyl)methoxy]-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



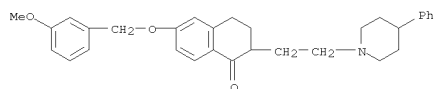
RN 212257-61-9 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-[(4-methylphenyl)methoxy]-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



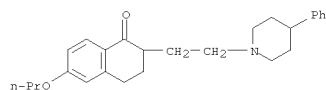
RN 212257-62-0 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-[(3-methoxyphenyl)methoxy]-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

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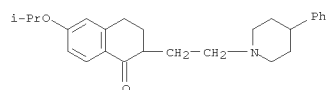
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
phenyl-1-piperidinylethyl]- (CA INDEX NAME)



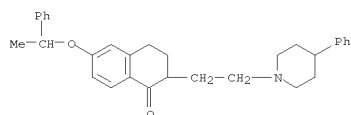
RN 212257-63-1 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[2-(4-phenyl-1-piperidinylethyl)-6-propoxy]- (CA INDEX NAME)



RN 212257-64-2 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-(1-methylethoxy)-2-[2-(4-phenyl-1-piperidinylethyl)- (CA INDEX NAME)

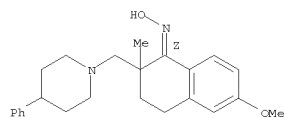


RN 212257-65-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-(1-phenylethoxy)-2-[2-(4-phenyl-1-piperidinylethyl)-, hydrochloride (1:1) (CA INDEX NAME)



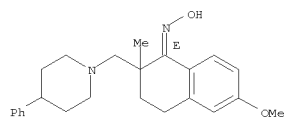
● HCl

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

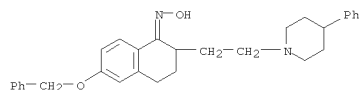


RN 212257-80-2 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-methyl-2-[(4-phenyl-1-piperidinylethyl)methyl]-, oxime, (1E)- (CA INDEX NAME)

Double bond geometry as shown.

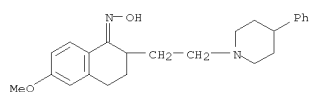


RN 212257-82-4 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-(phenylmethoxy)-2-[2-(4-phenyl-1-piperidinylethyl)-, oxime, hydrochloride (1:1) (CA INDEX NAME)



● HCl

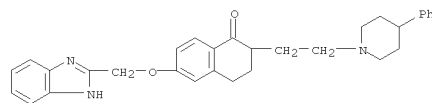
RN 212257-83-5 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[2-(4-phenyl-1-piperidinylethyl)-, oxime (CA INDEX NAME)



RN 212257-84-6 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[2-(4-phenyl-1-

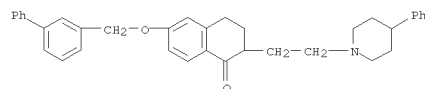
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

RN 212257-66-4 CAPLUS
CN 1(2H)-Naphthalenone, 6-(1H-benzimidazol-2-ylmethoxy)-3,4-dihydro-2-[2-(4-phenyl-1-piperidinylethyl)-, hydrochloride (1:2) (CA INDEX NAME)

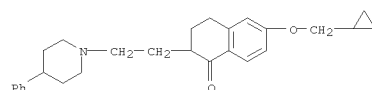


● 2 HCl

RN 212257-67-5 CAPLUS
CN 1(2H)-Naphthalenone, 6-([1,1'-biphenyl]-3-ylmethoxy)-3,4-dihydro-2-[2-(4-phenyl-1-piperidinylethyl)- (CA INDEX NAME)



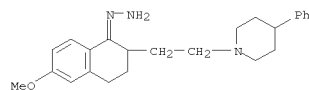
RN 212257-68-6 CAPLUS
CN 1(2H)-Naphthalenone, 6-(cyclopropylmethoxy)-3,4-dihydro-2-[2-(4-phenyl-1-piperidinylethyl)- (CA INDEX NAME)



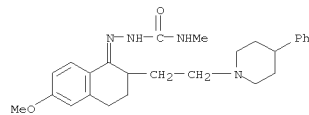
RN 212257-79-9 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-methyl-2-[(4-phenyl-1-piperidinylethyl)methyl]-, oxime, (1Z)- (CA INDEX NAME)

Double bond geometry as shown.

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
piperidinylethyl]-, hydrazone (CA INDEX NAME)

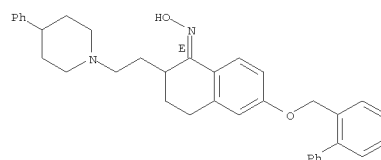


RN 212257-85-7 CAPLUS
CN Hydrazinecarboxamide, 2-[3,4-dihydro-6-methoxy-2-[2-(4-phenyl-1-piperidinylethyl)-1(2H)-naphthalenylidene]-N-methyl- (CA INDEX NAME)



RN 212257-86-8 CAPLUS
CN 1(2H)-Naphthalenone, 6-([1,1'-biphenyl]-2-ylmethoxy)-3,4-dihydro-2-[2-(4-phenyl-1-piperidinylethyl)-, oxime, (1E)- (CA INDEX NAME)

Double bond geometry as shown.

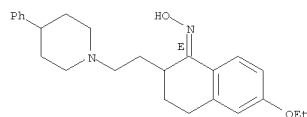


RN 212257-88-0 CAPLUS
CN 1(2H)-Naphthalenone, 6-ethoxy-3,4-dihydro-2-[2-(4-phenyl-1-piperidinylethyl)-, oxime, (1E)- (CA INDEX NAME)

Double bond geometry as shown.

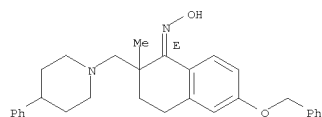
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L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



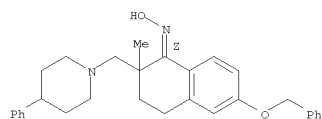
RN 212257-89-1 CAPLUS
CN 1(2H)-Naphthalenone,
3,4-dihydro-2-methyl-6-(phenylmethoxy)-2-[(4-phenyl-1-
piperidinyl)methyl]-, oxime, (1E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 212257-90-4 CAPLUS
CN 1(2H)-Naphthalenone,
3,4-dihydro-2-methyl-6-(phenylmethoxy)-2-[(4-phenyl-1-
piperidinyl)methyl]-, oxime, (1Z)- (CA INDEX NAME)

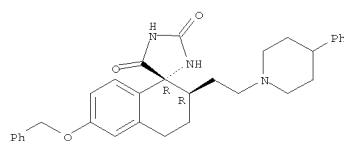
Double bond geometry as shown.



RN 212257-91-5 CAPLUS
CN Acetamide,
N-[(1R,2S)-1,2,3,4-tetrahydro-6-methoxy-2-methyl-2-[(4-phenyl-1-
piperidinyl)methyl]-1-naphthalenyl]-, rel- (CA INDEX NAME)

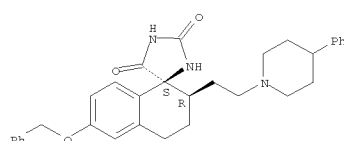
Relative stereochemistry.

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

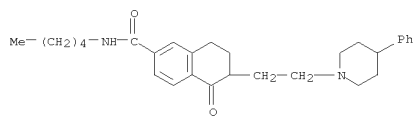


RN 212257-96-0 CAPLUS
CN Spiro[imidazolidine-4,1'(2'H)-naphthalene]-2,5-dione,
3',4'-dihydro-6'-(phenylmethoxy)-2'-[2-(4-phenyl-1-piperidinyl)ethyl]-,
(1'R,2'S)-rel- (CA INDEX NAME)

Relative stereochemistry.

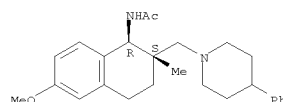


RN 212257-99-3 CAPLUS
CN 2-Naphthalenecarboxamide,
5,6,7,8-tetrahydro-5-oxo-N-pentyl-6-[2-(4-phenyl-1-
piperidinyl)ethyl]- (CA INDEX NAME)



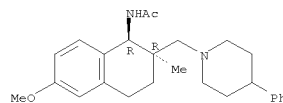
RN 212258-00-9 CAPLUS
CN 1(2H)-Naphthalenone,
3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]-6-(1-
piperidinylcarbonyl)- (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

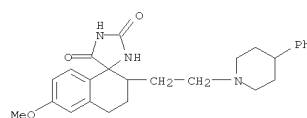


RN 212257-93-7 CAPLUS
CN Acetamide,
N-[(1R,2R)-1,2,3,4-tetrahydro-6-methoxy-2-methyl-2-[(4-phenyl-1-
piperidinyl)methyl]-1-naphthalenyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



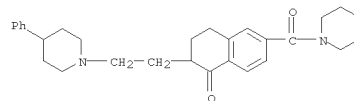
RN 212257-94-8 CAPLUS
CN Spiro[imidazolidine-4,1'(2'H)-naphthalene]-2,5-dione,
3',4'-dihydro-6'-(phenylmethoxy)-2'-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



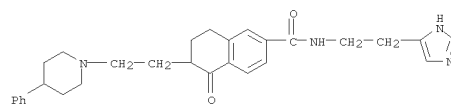
RN 212257-95-9 CAPLUS
CN Spiro[imidazolidine-4,1'(2'H)-naphthalene]-2,5-dione,
3',4'-dihydro-6'-(phenylmethoxy)-2'-[2-(4-phenyl-1-piperidinyl)ethyl]-,
(1'R,2'R)-rel- (CA INDEX NAME)

Relative stereochemistry.

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

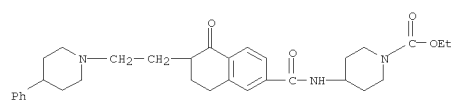


RN 212258-01-0 CAPLUS
CN 2-Naphthalenecarboxamide,
5,6,7,8-tetrahydro-N-[2-(1H-imidazol-5-yl)ethyl]-
5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

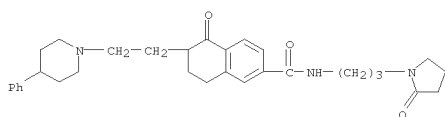
RN 212258-03-2 CAPLUS
CN 1-Piperidinecarboxylic acid,
4-[[[5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-
piperidinyl)ethyl]-2-naphthalenyl]carbonyl]amino]-, ethyl ester (CA INDEX NAME)



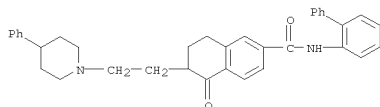
RN 212258-04-3 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-N-[3-(2-oxo-1-
pyrrolidinyl)propyl]-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

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L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

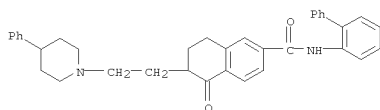


RN 212258-05-4 CAPLUS
CN 2-Naphthalenecarboxamide,
N-[1,1'-biphenyl]-2-yl-5,6,7,8-tetrahydro-5-oxo-
6-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)



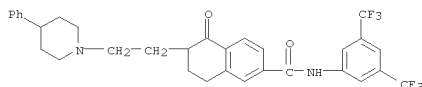
● HCl

RN 212258-06-5 CAPLUS
CN 2-Naphthalenecarboxamide,
N-[1,1'-biphenyl]-2-yl-5,6,7,8-tetrahydro-5-oxo-
6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



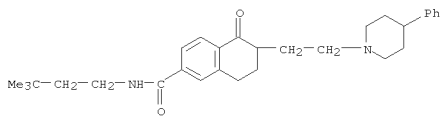
RN 212258-07-6 CAPLUS
CN 2-Naphthalenecarboxamide,
N-[1,1'-biphenyl]-2-yl-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



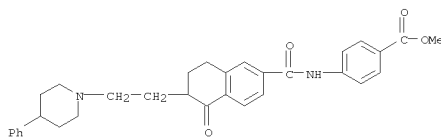
● HCl

RN 212258-11-2 CAPLUS
CN 2-Naphthalenecarboxamide,
N-(3,3-dimethylbutyl)-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)



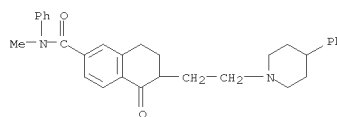
● HCl

RN 212258-12-3 CAPLUS
CN Benzoic acid, 4-[[[5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-2-naphthalenyl]carbonyl]amino]-, methyl ester (CA INDEX NAME)

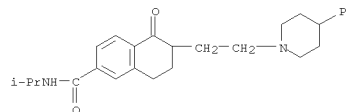


RN 212258-13-4 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-N-(2-methoxyphenyl)-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

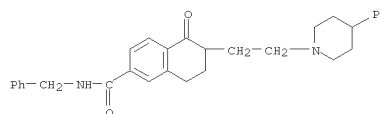
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 212258-08-7 CAPLUS
CN 2-Naphthalenecarboxamide,
5,6,7,8-tetrahydro-N-(1-methylethyl)-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

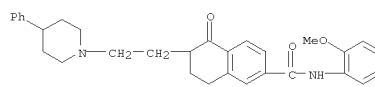


RN 212258-09-8 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-N-(phenylmethyl)-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



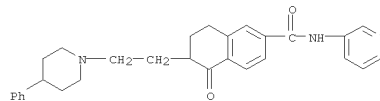
RN 212258-10-1 CAPLUS
CN 2-Naphthalenecarboxamide, N-[3,5-bis(trifluoromethyl)phenyl]-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



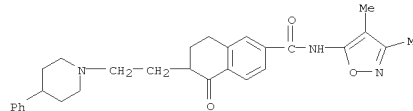
● HCl

RN 212258-14-5 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-N-3-pyridinyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 212258-15-6 CAPLUS
CN 2-Naphthalenecarboxamide,
N-(3,4-dimethyl-5-isoxazolyl)-5,6,7,8-tetrahydro-
5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

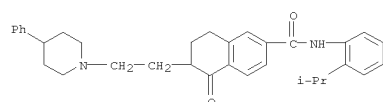


● HCl

RN 212258-16-7 CAPLUS
CN 2-Naphthalenecarboxamide,
5,6,7,8-tetrahydro-N-[2-(1-methylethyl)phenyl]-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

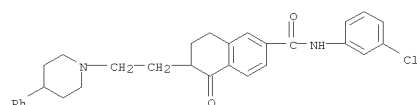
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L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



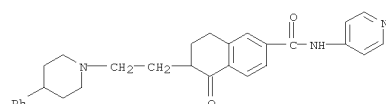
● HCl

RN 212258-17-8 CAPLUS
CN 2-Naphthalenecarboxamide,
N-(3-chlorophenyl)-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

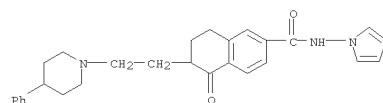
RN 212258-18-9 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-N-4-pyridinyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

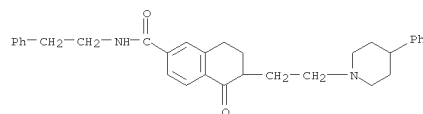
RN 212258-19-0 CAPLUS
CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, 1-phenylhydrazide, hydrochloride (1:2) (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

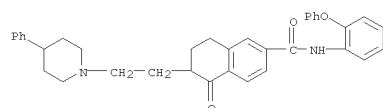


● HCl

RN 212258-25-8 CAPLUS
CN 2-Naphthalenecarboxamide,
5,6,7,8-tetrahydro-5-oxo-N-(2-phenylethyl)-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



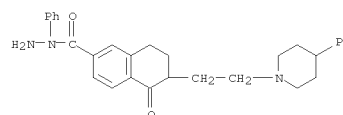
RN 212258-26-9 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-N-(2-phenoxypheyl)-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

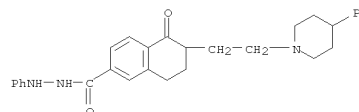
RN 212258-27-0 CAPLUS
CN 2-Naphthalenecarboxamide,
N-(3,5-dimethoxyphenyl)-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



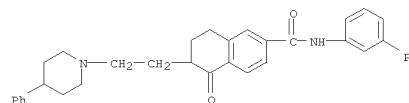
● 2 HCl

RN 212258-20-3 CAPLUS
CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, 2-phenylhydrazide, hydrochloride (4:5) (CA INDEX NAME)



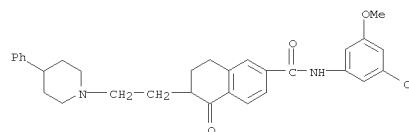
● 5/4 HCl

RN 212258-23-6 CAPLUS
CN 2-Naphthalenecarboxamide,
N-[1,1'-biphenyl]-3-yl-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



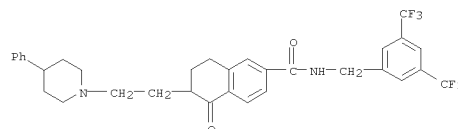
RN 212258-24-7 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-N-1H-pyrrol-1-yl-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



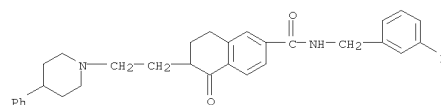
● HCl

RN 212258-29-2 CAPLUS
CN 2-Naphthalenecarboxamide, N-([3,5-bis(trifluoromethyl)phenyl]methyl)-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 212258-30-5 CAPLUS
CN 2-Naphthalenecarboxamide, N-([1,1'-biphenyl]-3-ylmethyl)-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

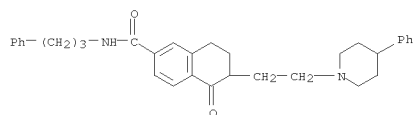


● HCl

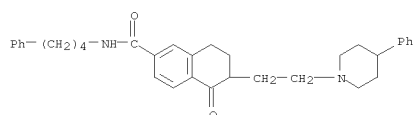
RN 212258-31-6 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-

10590585.trn

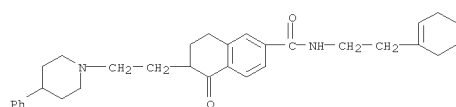
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
piperidinylethyl]-N-(3-phenylpropyl)- (CA INDEX NAME)



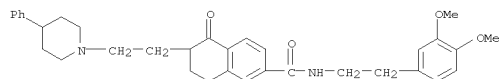
RN 212258-32-7 CAPLUS
CN 2-Naphthalenecarboxamide,
N-(2,2-diphenylethyl)-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



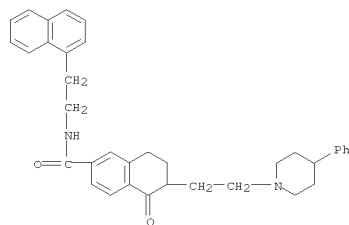
RN 212258-33-8 CAPLUS
CN 2-Naphthalenecarboxamide, N-[2-(1-cyclohexen-1-yl)ethyl]-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212258-34-9 CAPLUS
CN 2-Naphthalenecarboxamide, N-[2-(3,4-dimethoxyphenyl)ethyl]-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

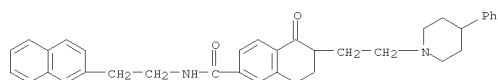


L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

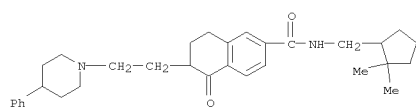


● HCl

RN 212258-38-3 CAPLUS
CN 2-Naphthalenecarboxamide,
5,6,7,8-tetrahydro-N-[2-(2-naphthalenyl)ethyl]-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212258-39-4 CAPLUS
CN 2-Naphthalenecarboxamide, N-[(2,2-dimethylcyclopentyl)methyl]-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

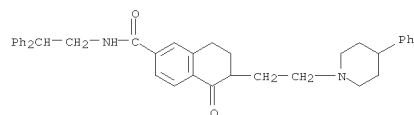


RN 212258-40-7 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-N-[(1R,2S)-2-phenylcyclopropyl]-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, rel- (CA INDEX NAME)

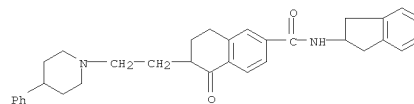
Relative stereochemistry.

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

RN 212258-35-0 CAPLUS
CN 2-Naphthalenecarboxamide,
N-(2,2-diphenylethyl)-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

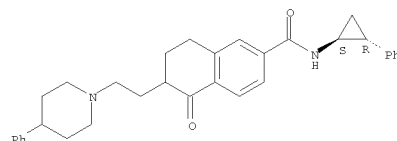


RN 212258-36-1 CAPLUS
CN 2-Naphthalenecarboxamide,
N-(2,3-dihydro-1H-inden-2-yl)-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

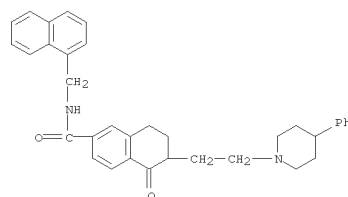


RN 212258-37-2 CAPLUS
CN 2-Naphthalenecarboxamide,
5,6,7,8-tetrahydro-N-[2-(1-naphthalenyl)ethyl]-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

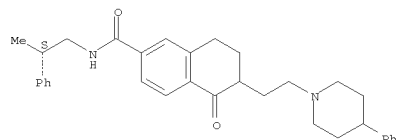


RN 212258-41-8 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-N-(1-naphthalenylmethyl)-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212258-42-9 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-N-[(2S)-2-phenylpropyl]- (CA INDEX NAME)

Absolute stereochemistry.

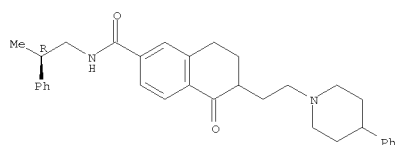


RN 212258-43-0 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-N-[(2R)-2-phenylpropyl]- (CA INDEX NAME)

Absolute stereochemistry.

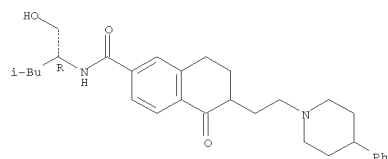
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L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



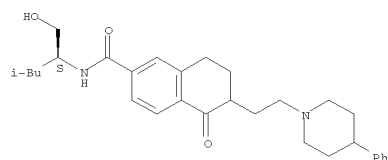
RN 212258-44-1 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-N-[(1R)-1-(hydroxymethyl)-3-methylbutyl]-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



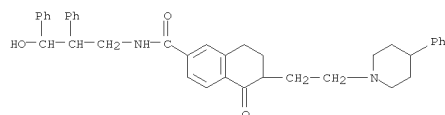
RN 212258-45-2 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-N-[(1S)-1-(hydroxymethyl)-3-methylbutyl]-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



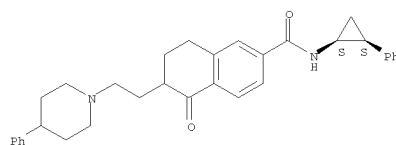
RN 212258-46-3 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-N-[2-(2-thienyl)ethyl]- (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

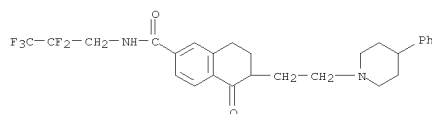


RN 212258-50-9 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-N-[(1R,2R)-2-phenylcyclopropyl]-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



RN 212258-51-0 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-N-(2,2,3,3,3-pentafluoropropyl)-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

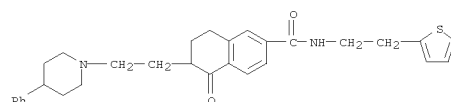


RN 212258-53-2 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-N-(2-methylbutyl)-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

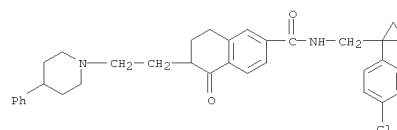
CM 1

CRN 212258-52-1
CMF C29 H38 N2 O2

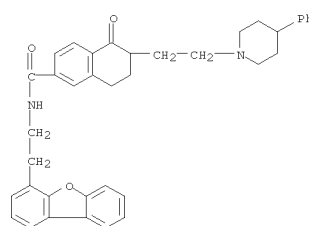
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 212258-47-4 CAPLUS
CN 2-Naphthalenecarboxamide, N-[1-(4-chlorophenyl)cyclopropylmethyl]-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

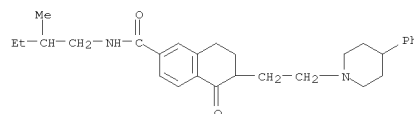


RN 212258-48-5 CAPLUS
CN 2-Naphthalenecarboxamide, N-[2-(4-dibenzofuranyl)ethyl]-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212258-49-6 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-N-(3-hydroxy-2,3-diphenylpropyl)-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 2

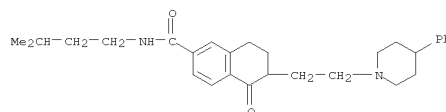
CRN 76-05-1
CMF C2 H F3 O2



RN 212258-55-4 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-N-(3-methylbutyl)-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 212258-54-3
CMF C29 H38 N2 O2



CM 2

CRN 76-05-1
CMF C2 H F3 O2

10590585.trn

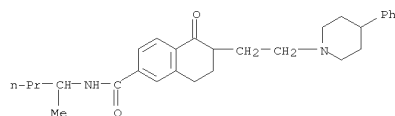
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 212258-57-6 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-N-(1-methylbutyl)-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 212258-56-5
CMF C29 H38 N2 O2



CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 212258-59-8 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-N-[(tetrahydro-2-furanyl)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 212258-58-7
CMF C29 H36 N2 O3

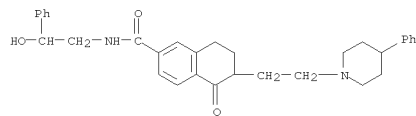
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 212258-63-4 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-N-(2-hydroxy-2-phenylethyl)-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 212258-62-3
CMF C32 H36 N2 O3



CM 2

CRN 76-05-1
CMF C2 H F3 O2

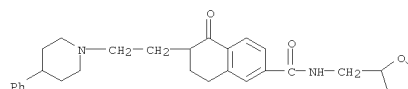


RN 212258-65-6 CAPLUS
CN 2-Naphthalenecarboxamide, N-[2-(2-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 212258-64-5
CMF C32 H35 F N2 O2

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 2

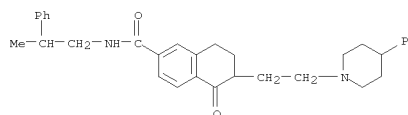
CRN 76-05-1
CMF C2 H F3 O2



RN 212258-61-2 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-N-(2-phenylpropyl)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

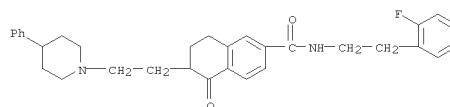
CRN 212258-60-1
CMF C33 H38 N2 O2



CM 2

CRN 76-05-1
CMF C2 H F3 O2

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 2

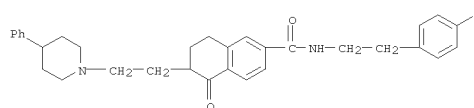
CRN 76-05-1
CMF C2 H F3 O2



RN 212258-67-8 CAPLUS
CN 2-Naphthalenecarboxamide, N-[2-(4-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 212258-66-7
CMF C32 H35 F N2 O2



CM 2

CRN 76-05-1
CMF C2 H F3 O2

10590585.trn

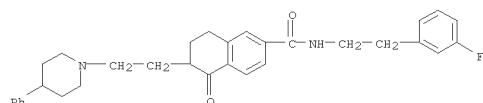
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 212258-69-0 CAPLUS
CN 2-Naphthalenecarboxamide,
N-[2-(3-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-5-
oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, 2,2,2-trifluoroacetate (1:1)
(CA INDEX NAME)

CM 1

CRN 212258-68-9
CMF C32 H35 F N2 O2



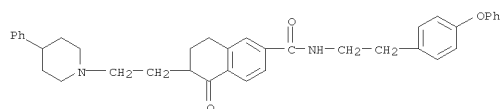
CM 2

CRN 76-05-1
CMF C2 H F3 O2

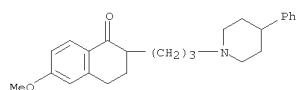


RN 212258-70-3 CAPLUS
CN 2-Naphthalenecarboxamide,
N-[2-(4-chlorophenyl)ethyl]-5,6,7,8-tetrahydro-5-
oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

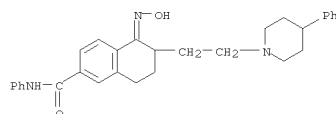


RN 212258-75-8 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[3-(4-phenyl-1-
piperidinyl)propyl]-, hydrochloride (1:1) (CA INDEX NAME)

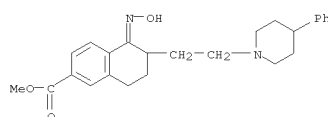


● HCl

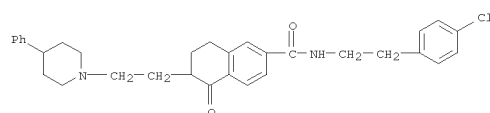
RN 212258-78-1 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-(hydroxyimino)-N-phenyl-6-
[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



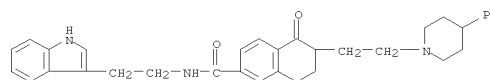
RN 212258-79-2 CAPLUS
CN 2-Naphthalenecarboxylic acid,
5,6,7,8-tetrahydro-5-(hydroxyimino)-6-[2-(4-
phenyl-1-piperidinyl)ethyl]-, methyl ester (CA INDEX NAME)



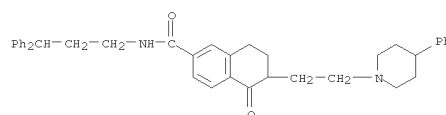
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 212258-72-5 CAPLUS
CN 2-Naphthalenecarboxamide,
N-[2-(1H-indol-3-yl)ethyl]-5-
oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



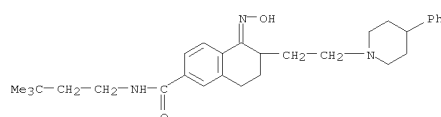
RN 212258-73-6 CAPLUS
CN 2-Naphthalenecarboxamide,
N-(3,3-diphenylpropyl)-5,6,7,8-tetrahydro-5-oxo-
6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



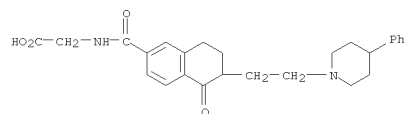
RN 212258-74-7 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-N-[2-(4-
phenoxyphenyl)ethyl]-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX
NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

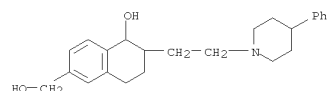
RN 212258-81-6 CAPLUS
CN 2-Naphthalenecarboxamide, N-(3,3-dimethylbutyl)-5,6,7,8-tetrahydro-5-
(hydroxyimino)-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212258-82-7 CAPLUS
CN Glycine,
N-[5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-
2-naphthalenyl]carbonyl]- (CA INDEX NAME)



RN 212258-83-8 CAPLUS
CN 2-Naphthalenemethanol, 5,6,7,8-tetrahydro-5-hydroxy-6-[2-(4-phenyl-1-
piperidinyl)ethyl]- (CA INDEX NAME)



RN 212258-85-0 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-hydroxy-N-phenyl-6-[2-(4-
phenyl-1-piperidinyl)ethyl]-, (5R,6S)-rel-, 2,2,2-trifluoroacetate (1:1)
(CA INDEX NAME)

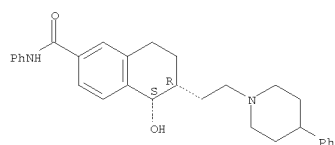
CM 1

CRN 212258-84-9
CMF C30 H34 N2 O2

Relative stereochemistry.

10590585.trn

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

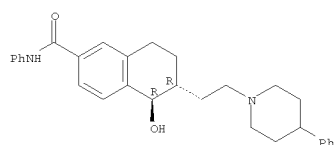


RN 212258-87-2 CAPLUS
CN 2-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-hydroxy-N-phenyl-6-[2-(4-phenyl-1-piperidinyl)ethyl]-, (5R,6R)-rel-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 212258-86-1
CMF C30 H34 N2 O2

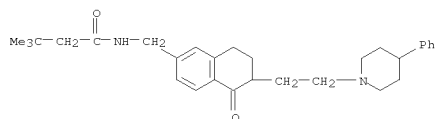
Relative stereochemistry.



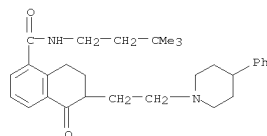
CM 2

CRN 76-05-1

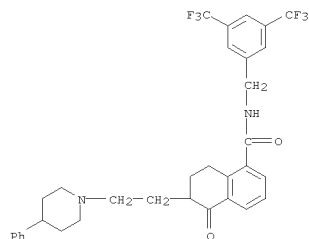
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 212258-97-4 CAPLUS
CN 1-Naphthalenecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212258-98-5 CAPLUS
CN 1-Naphthalenecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

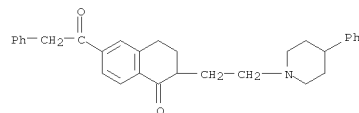


RN 212258-99-6 CAPLUS
CN 1-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-N-(phenylmethyl)-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

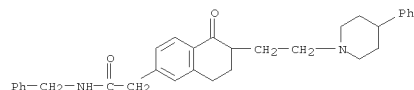
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
CMF C2 H F3 O2



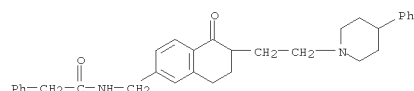
RN 212258-89-4 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-(2-phenylacetyl)-2-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212258-90-7 CAPLUS
CN 2-Naphthaleneacetamide, 5,6,7,8-tetrahydro-5-oxo-N-(phenylmethyl)-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

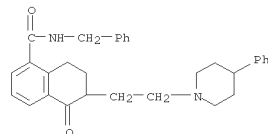


RN 212258-91-8 CAPLUS
CN Benzeneacetamide, N-[[5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-2-naphthalenyl]methyl]- (CA INDEX NAME)

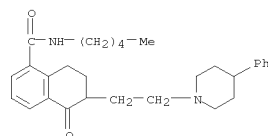


RN 212258-92-9 CAPLUS
CN Butanamide, 3,3-dimethyl-N-[[5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-2-naphthalenyl]methyl]- (CA INDEX NAME)

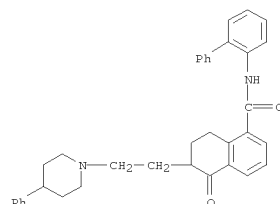
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 212259-00-2 CAPLUS
CN 1-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-N-pentyl-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212259-01-3 CAPLUS
CN 1-Naphthalenecarboxamide, N-[1,1'-biphenyl]-2-yl-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



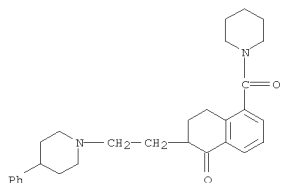
RN 212259-03-5 CAPLUS
CN Piperidine, 1-[[5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-1-naphthalenyl]carbonyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

10590585.trn

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

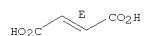
CRN 212259-02-4
CMF C29 H36 N2 O2



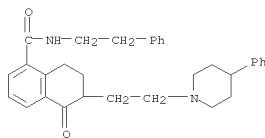
CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

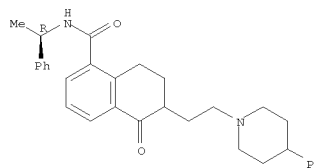


RN 212259-04-6 CAPLUS
CN 1-Naphthalenecarboxamide,
5,6,7,8-tetrahydro-5-oxo-N-[(1S)-1-phenylethyl]-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



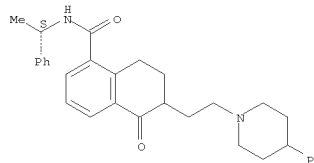
RN 212259-05-7 CAPLUS
CN 1-Naphthalenecarboxamide,
5,6,7,8-tetrahydro-5-oxo-N-[(1R)-1-phenylethyl]-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
Absolute stereochemistry.



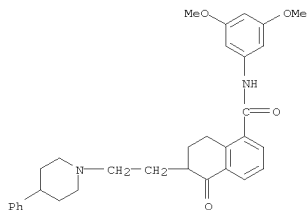
RN 212259-06-8 CAPLUS
CN 1-Naphthalenecarboxamide,
5,6,7,8-tetrahydro-5-oxo-N-[(1S)-1-phenylethyl]-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

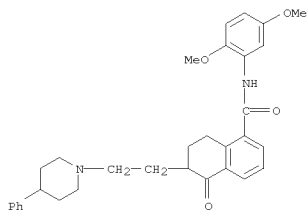


RN 212259-07-9 CAPLUS
CN 1-Naphthalenecarboxamide,
N-(3,5-dimethoxyphenyl)-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

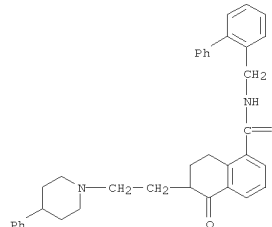


RN 212259-08-0 CAPLUS
CN 1-Naphthalenecarboxamide,
N-(2,5-dimethoxyphenyl)-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

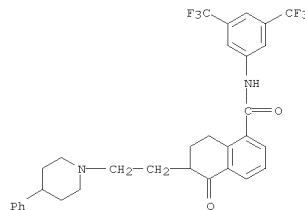


RN 212259-09-1 CAPLUS
CN 1-Naphthalenecarboxamide, N-([1,1'-biphenyl]-2-ylmethyl)-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



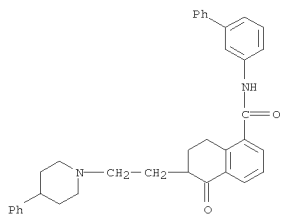
RN 212259-10-4 CAPLUS
CN 1-Naphthalenecarboxamide, N-[3,5-bis(trifluoromethyl)phenyl]-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



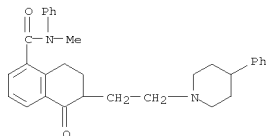
RN 212259-11-5 CAPLUS
CN 1-Naphthalenecarboxamide,
N-[1,1'-biphenyl]-3-yl-5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

10590585.trn

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

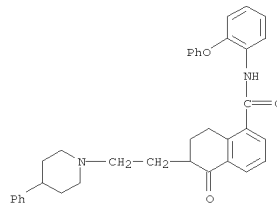


RN 212259-12-6 CAPLUS
CN 1-Naphthalenecarboxamide,
5,6,7,8-tetrahydro-N-methyl-5-oxo-N-phenyl-6-[2-
(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

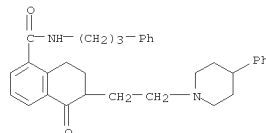


RN 212259-13-7 CAPLUS
CN 1-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-N-(2-phenoxyphenyl)-6-
[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

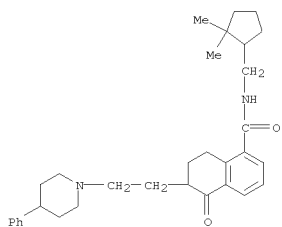


RN 212259-14-8 CAPLUS
CN 1-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-
piperidinyl)ethyl]-N-(3-phenylpropyl)- (CA INDEX NAME)

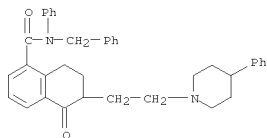


RN 212259-15-9 CAPLUS
CN 1-Naphthalenecarboxamide, N-[(2,2-dimethylcyclopentyl)methyl]-5,6,7,8-
tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

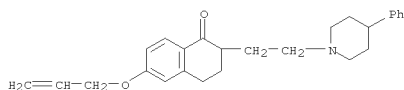
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 212259-16-0 CAPLUS
CN 1-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-oxo-N-phenyl-N-
(phenylmethyl)-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

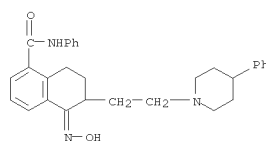


RN 212259-64-8 CAPLUS
CN 1(2H)-Naphthalenone,
3,4-dihydro-2-[2-(4-phenyl-1-piperidinyl)ethyl]-6-(2-
propen-1-yloxy)- (CA INDEX NAME)



RN 212260-11-2 CAPLUS
CN 1-Naphthalenecarboxamide, 5,6,7,8-tetrahydro-5-(hydroxyimino)-N-phenyl-6-
[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

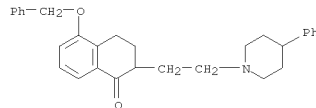


RN 212330-98-8 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-5-(phenylmethoxy)-2-[2-(4-phenyl-1-
piperidinyl)ethyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 212330-97-7

CMF C30 H33 N O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2

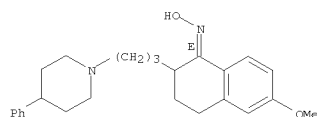


RN 212330-99-9 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[3-(4-phenyl-1-
piperidinyl)propyl]-, oxime, (1E)- (CA INDEX NAME)

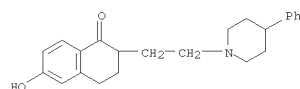
Double bond geometry as shown.

10590585.trn

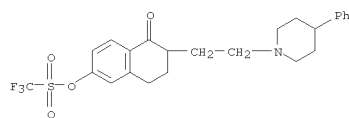
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



IT 212259-30-8P 212259-31-9P 212259-32-0P
 212259-33-1P 212259-34-2P 212259-40-0P
 212259-45-5P 212259-46-6P 212259-47-7P
 212259-48-8P 212259-49-9P 212259-50-2P
 212259-51-3P 212259-57-9P 212259-58-0P
 212259-59-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of tetralones as antiarrhythmic agents)
 RN 212259-30-8 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-hydroxy-2-[2-(4-phenyl-1-
 piperidinyl)ethyl]- (CA INDEX NAME)

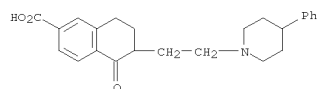


RN 212259-31-9 CAPLUS
 CN Methanesulfonic acid, 1,1,1-trifluoro-,
 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]-2-
 naphthalenyl ester (CA INDEX NAME)



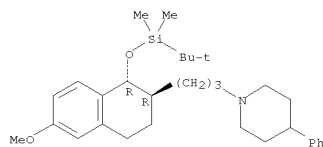
RN 212259-32-0 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-(2-phenylethynyl)-2-[2-(4-phenyl-1-
 piperidinyl)ethyl]- (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

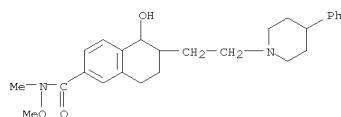


RN 212259-45-5 CAPLUS
 CN Piperidine, 1-[3-[(1R,2R)-1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-
 1,2,3,4-tetrahydro-6-methoxy-2-naphthalenyl]propyl]-4-phenyl-, rel- (CA
 INDEX NAME)

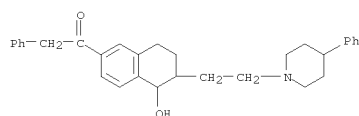
Relative stereochemistry.



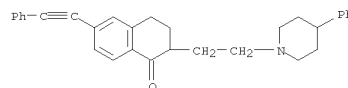
RN 212259-46-6 CAPLUS
 CN 2-Naphthalenecarboxamide,
 5,6,7,8-tetrahydro-5-hydroxy-N-methoxy-N-methyl-
 6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



RN 212259-47-7 CAPLUS
 CN Ethanone, 2-phenyl-1-[5,6,7,8-tetrahydro-5-hydroxy-6-[2-(4-phenyl-1-
 piperidinyl)ethyl]-2-naphthalenyl]- (CA INDEX NAME)

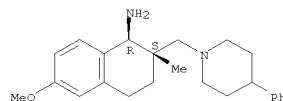


L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 212259-33-1 CAPLUS
 CN 1-Naphthalenamine, 1,2,3,4-tetrahydro-6-methoxy-2-methyl-2-[(4-phenyl-1-
 piperidinyl)methyl]-, hydrochloride (1:2), (1R,2S)-rel- (CA INDEX NAME)

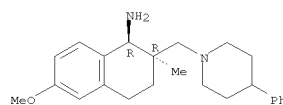
Relative stereochemistry.



● 2 HCl

RN 212259-34-2 CAPLUS
 CN 1-Naphthalenamine, 1,2,3,4-tetrahydro-6-methoxy-2-methyl-2-[(4-phenyl-1-
 piperidinyl)methyl]-, hydrochloride (1:1), (1R,2R)-rel- (CA INDEX NAME)

Relative stereochemistry.

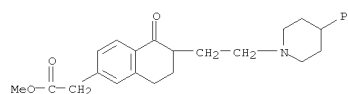


● HCl

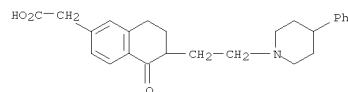
RN 212259-40-0 CAPLUS
 CN 2-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-
 piperidinyl)ethyl]- (CA INDEX NAME)

L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

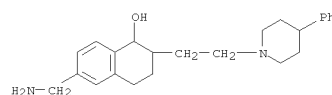
RN 212259-48-8 CAPLUS
 CN 2-Naphthaleneacetic acid, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-
 piperidinyl)ethyl]-, methyl ester (CA INDEX NAME)



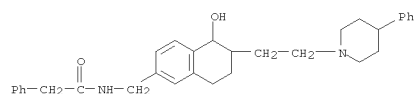
RN 212259-49-9 CAPLUS
 CN 2-Naphthaleneacetic acid, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-
 piperidinyl)ethyl]- (CA INDEX NAME)



RN 212259-50-2 CAPLUS
 CN 1-Naphthalenol, 6-(aminomethyl)-1,2,3,4-tetrahydro-2-[2-(4-phenyl-1-
 piperidinyl)ethyl]- (CA INDEX NAME)



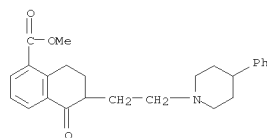
RN 212259-51-3 CAPLUS
 CN Benzeneacetamide, N-[[[5,6,7,8-tetrahydro-5-hydroxy-6-[2-(4-phenyl-1-
 piperidinyl)ethyl]-2-naphthalenyl]methyl]- (CA INDEX NAME)



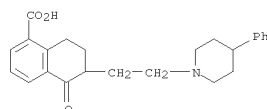
RN 212259-57-9 CAPLUS
 CN 1-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-
 piperidinyl)ethyl]-, methyl ester (CA INDEX NAME)

10590585.trn

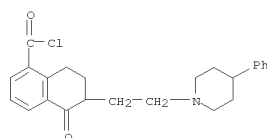
L25 ANSWER 55 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 212259-58-0 CAPLUS
CN 1-Naphthalenecarboxylic acid, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



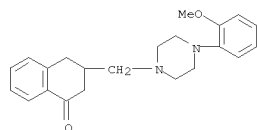
RN 212259-59-1 CAPLUS
CN 1-Naphthalenecarbonyl chloride, 5,6,7,8-tetrahydro-5-oxo-6-[2-(4-phenyl-1-piperidinyl)ethyl]- (CA INDEX NAME)



L25 ANSWER 57 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1998:236274 Document No. 128:2827800 Original Reference No.
128:55978h,55979a Preparation of heterocyclic inhibitors of microsomal triglyceride transfer protein. Biller, Scott A.; Dickson, John K.; Lawrence, R. Michael; Magnin, David R.; Posa, Michael A.; Sulsky, Richard B.; Tino, Joseph A. (Bristol-Myers Squibb Co., USA). U.S. US 5739135 A 19980414, 185 pp., Cont.-in-part of U.S. Ser. No. 391,901, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1995-472067 19950606. PRIORITY: US 1993-117362 19930903; US 1994-284808 19940805; US 1995-391901 19950221.
GI

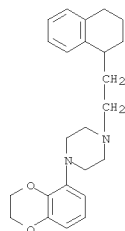
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I-V; Q = C(O), S(O)2; X = CHR8, C(O), CHR9CHR10, CR9:CR10 (wherein R8-R10 = H, alkyl, alkenyl, etc.); Y = (CH2)m, C(O) (m = 2-3); R1 = alkyl, alkenyl, alkynyl, etc.; R2-R4 = H, halo, alkyl, etc.; R5 = alkyl, alkenyl, alkynyl, etc.; R6 = H, C1-4 alkyl, C1-4 alkenyl] which inhibit microsomal triglyceride transfer protein and thus are useful for lowering serum lipids and treating atherosclerosis and related diseases such as hyperglycemia and obesity, were prepared Thus, reaction of 1-(3,3-diphenylpropyl)-4-piperidinamine.HCl (preparation described) with benzoyl chloride in the presence of Et3N in CH2Cl2 afforded 84% the title compound III.HCl [Q = C(O); R1 = 3,3-diphenylpropyl; R5 = Ph; R6 = H]. Compds. I-V are effective at 5-500 mg/day.
IT 133496-73-8P 163266-60-2P 205931-38-0P
205931-39-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of heterocyclic inhibitors of microsomal triglyceride transfer protein)
RN 133496-73-8 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-, hydrochloride (1:2) (CA INDEX NAME)

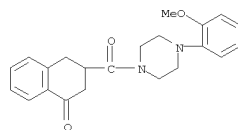


● 2 HCl

L25 ANSWER 56 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1998:349268 Document No. 129:62433 Original Reference No. 129:12769a
Theoretical descriptors in quantitative structure-affinity and selectivity relationship study of potent N4-substituted arylpiperazine 5-HT1A receptor antagonists. Menziani, M. C.; De Benedetti, P. G.; Karelson, M. (Dipartimento di Chimica, Universita' di Modena, Modena, 41100, Italy). Bioorganic & Medicinal Chemistry, 6(5), 535-550 (English) 1998. CODEN: BMCEP. ISSN: 0968-0896. Publisher: Elsevier Science Ltd..
AB The ability of ad hoc defined size and shape descriptors and theor. descriptors derived on a single structure to give powerful interpretative and predictive QSAR models was compared and evaluated with respect to the quality of the pharmacol. data available for structurally diverse 5-HT1A receptor antagonists, displaying selectivity towards the α1-adrenergic receptor.
IT 143355-89-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); CAT (Catalyst use); PEP (Physical, engineering or chemical process); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses) (theor. descriptors in QSAR study of arylpiperazine 5-HT1A receptor antagonists)
RN 143355-89-9 CAPLUS
CN Piperazine, 1-(2,3-dihydro-1,4-benzodioxin-5-yl)-4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]- (CA INDEX NAME)

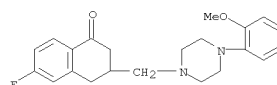


L25 ANSWER 57 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
RN 163266-60-2 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[[4-(2-methoxyphenyl)-1-piperazinyl]carbonyl]-, hydrochloride (1:1) (CA INDEX NAME)

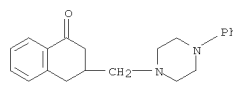


● HCl

RN 205931-38-0 CAPLUS
CN 1(2H)-Naphthalenone, 6-fluoro-3,4-dihydro-3-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



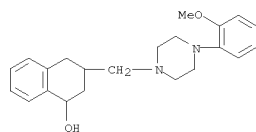
RN 205931-39-1 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[[4-(phenyl-1-piperazinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



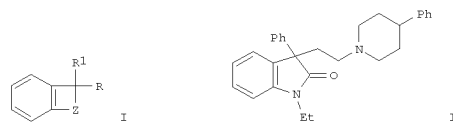
● HCl

IT 163268-03-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of heterocyclic inhibitors of microsomal triglyceride transfer protein)
RN 163268-03-9 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-3-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)

L25 ANSWER 57 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

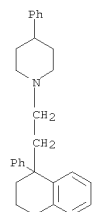


L25 ANSWER 58 of 96 CAPLUS COPYRIGHT 2010 ACS on STN
1998:71131 Document No. 128:1407290 Original Reference No.
128:27691a,27694a
Preparation of 3-[2-(4-arylazino)ethyl]-2-indolones and analogs as
antoincintinence agents. Kato, Kaneoyoshi; Doi, Takayuki; Sugiura,
Yoshihiro; Kawada, Mitsuru (Takeda Chemical Industries, Ltd., Japan).
PCT Int. Appl. WO 9802434 A1 19980122, 185 pp. DESIGNATED STATES: W: AL,
AM,
AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, KG, KP,
KZ, LK, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RU, SG, SI,
SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, BG, KZ, MD, RU,
TJ, TM, TR, UA, BE, AF, BE, BF, BF, CF, CG, CH, CI, CM, DE, DK, ES, FI, FG, GA,
GB, GR, IE, IT, LU, MC, ML, MR, NE, NP, ET, SE, SN, TD, TG. (English)
CODEN: PIXDK2. APPLICATION: NO 1997-172447 19970715. PRIORITY: JP
1996-186025 19960716; JP 1997-87980 19970407.



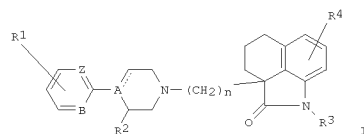
AB	Title compds. (ring-substituted) I; R = (CH ₂) _m 122R ₂ ; R ₁ ,R ₂ = (un)substituted aryl; Z = atoms to complete a (heterocyclic) ring; Z1 = (un)substituted N-attached heterocycliclylene; Z2 = bond or (oxo)alkylene; m = 1-3) were prepared. Thus, PhCH ₂ OCH ₂ Et was arylated by 4-PC ₆ H ₄ NO ₂ and the cyclized product converted in 3 steps to title compound II. Data for biol. activity of I were given.
IT	202260-59-1P
(Biological	RL: BAC (Biological activity or effector, except adverse); BSU study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PRFP (Preparation); USES (Uses)
	[Preparation of 3-(2-(4-arylazino)ethyl)-2-indolones and analogs as antineoplastic agents]
RN	202260-59-1 CAPLUS
CN	Piperidine, 4-phenyl-1-[2-(1,2,3,4-tetrahydro-1-phenyl-1-naphthalenyl)ethyl]-, hydrochloride (1:1). (CA INDEX NAME)

L25 ANSWER 58 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● HCl

125 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1998:55616 Document No. 128:1149610 Original Reference No.
128:225414, 22544a
Preparation of tetrahydrobenzindole derivatives for the treatment or
prevention of mental diseases. Koyama, Masao; Kikuchi, Chika; Ushiroda,
Osamu; Ando, Takashi; Nagao, Hiroshi; Fujii, Kazuyuki; Okuno, Masayo;
Hiranuma, Toyokazu (Meiji Seika Kaisha, Ltd., Japan). PCT Int. Appl. WO
9800400 A1 19980108, 67 pp. DESIGNATED STATES: W: CA, JP, NO, US; RW:
AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE.
[Japanese]. CODEN: FIMX2D. APPLICATION: WO 1997-JP2226 19970627.
JPH082471 JP 1996-0418; JP 1997-96271 19970415; JP 1997-130201
19970521; JP 1997-144376 19970603.



AB	The title compds. I [A represents N, CH, C having a double bond or CR5; B and Z independently represent each N, CH or CR1, provided that A is N when		
	B and/or Z is N; R1 represents hydrogen, halogeno, lower alkyl, cyano, trihalomethyl, hydroxy, alkoxy, alkylthio, alkylsulfenyl, alkylsulfonyl, alkoxy carbonyl, sulfamoyl, optionally substituted amino, optionally alkylated carbamoyl, acyl or carboxy; R2 represents hydrogen or lower alkyl; R3 represents hydrogen, lower alkyl; R3 represents hydrogen, lower alkyl or aralkyl; R4 represents hydrogen, halogeno, lower alkyl, hydroxyl,		
	alkoxy, acyl, alkoxy carbonyl, nitro, optionally substituted amino, optionally alkylated carbamoyl or acyloxy; R5 represents lower alkyl, cyano, carbamoyl, carboxy, acyl, acyloxy, alkoxy, alkoxy carbonyl, trihalomethyl or hydroxy; and n is an integer of from 2 to 6] are		
prepared	I strongly inhibit [3H]-serotonin and [3H]-5-CT binding to the human serotonin 5-HT7 receptor subtype expressed in a cultured cell line and		
are	useful for treating or preventing mental diseases.		
	2a-[4-{4-(2-methoxyphenyl)piperazinyl}butyl]-2a,3,4,5-tetrahydrobenzo[cd]indol-2-(1H)-one was prepared from 2a,3,4,5-tetrahydrobenzo[cd]indol-2-(1H)-one. In tests for affinity for the 5-HT7 receptors, compds. of this invention showed Ki values of 8.9 nM to 27 nM. The title compds. showed selective affinity for 5-HT7 receptors.		
IT	201608-38-0P	201608-39-1P	201608-42-6P
	201608-43-7P	201608-44-8P	201608-45-9P
	201608-46-0P	201608-47-1P	201608-48-2P
	201608-49-3P	201608-50-6P	201608-51-7P
	201608-52-8P	201608-53-9P	201608-54-0P
	201608-55-1P	201608-56-2P	201608-57-3P
	201608-58-4P	201608-59-5P	201608-60-8P
	201608-61-9P	201608-64-2P	201608-65-3P

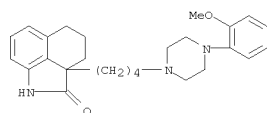
10590585.trn

L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

201608-68-6P 201608-69-7P 201608-70-0P
201608-75-5P 201608-76-6P 201608-77-7P
201608-78-8P 201608-79-9P 201608-80-2P
201608-81-3P 201608-82-4P 201608-83-5P
201608-84-6P 201608-85-7P 201608-86-8P
201608-87-9P 201608-88-0P 201608-89-1P
201608-90-4P 201608-91-5P 201608-92-6P
201608-93-7P 201608-94-8P 201608-95-9P
201608-96-0P 201608-97-1P 201608-98-2P
201608-99-3P 201609-01-0P 201609-03-2P
201609-06-5P 201609-07-6P 201609-11-2P
201609-14-5P 201609-16-7P 201609-18-9P
201609-20-3P 201609-21-4P 201609-22-5P
201609-23-6P 201609-24-7P

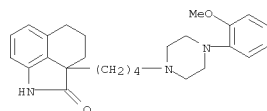
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of tetrahydrobenzindole derivs. for treatment or prevention of mental diseases)

RN 201608-38-0 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-, hydrochloride (1:1) (CA INDEX NAME)



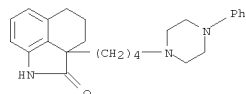
● HCl

RN 201608-39-1 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)

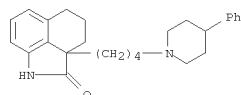


L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

piperazinyl]butyl]- (CA INDEX NAME)

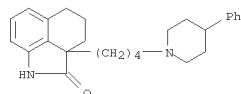


RN 201608-46-0 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-phenyl-1-piperidinyl)butyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

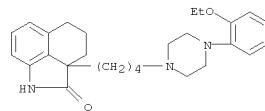
RN 201608-47-1 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-phenyl-1-piperidinyl)butyl]- (CA INDEX NAME)



RN 201608-48-2 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(4-methoxyphenyl)-1-piperazinyl]butyl]-, hydrochloride (1:1) (CA INDEX NAME)

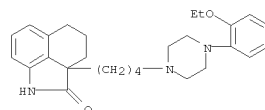
L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

RN 201608-42-6 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a-[4-[4-(2-ethoxyphenyl)-1-piperazinyl]butyl]- 2a,3,4,5-tetrahydro-, hydrochloride (1:1) (CA INDEX NAME)

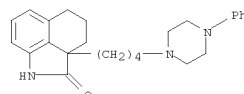


● HCl

RN 201608-43-7 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a-[4-[4-(2-ethoxyphenyl)-1-piperazinyl]butyl]- 2a,3,4,5-tetrahydro- (CA INDEX NAME)



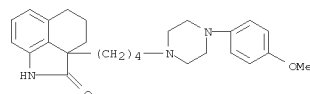
RN 201608-44-8 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-phenyl-1-piperazinyl)butyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

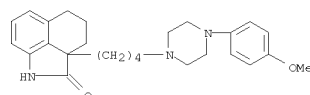
RN 201608-45-9 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-phenyl-1-

L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

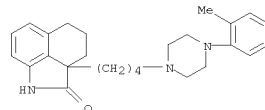


● HCl

RN 201608-49-3 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(4-methoxyphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



RN 201608-50-6 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-methylphenyl)-1-piperazinyl]butyl]-, hydrochloride (1:1) (CA INDEX NAME)

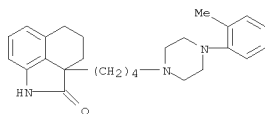


● HCl

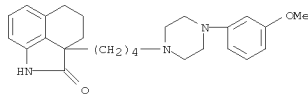
RN 201608-51-7 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-methylphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)

10590585.trn

L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

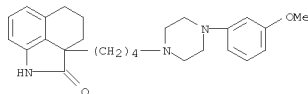


RN 201608-52-8 CAPLUS
CN Benz[cd]indol-2(1H)-one,
2a,3,4,5-tetrahydro-2a-[4-[4-(3-methoxyphenyl)-1-
piperazinyl]butyl]-, hydrochloride (1:1) (CA INDEX NAME)



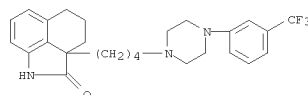
● HCl

RN 201608-53-9 CAPLUS
CN Benz[cd]indol-2(1H)-one,
2a,3,4,5-tetrahydro-2a-[4-[4-(3-methoxyphenyl)-1-
piperazinyl]butyl]- (CA INDEX NAME)



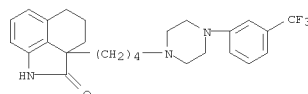
RN 201608-54-0 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-[3-
(trifluoromethyl)phenyl]-1-piperazinyl]butyl]-, hydrochloride (1:1) (CA
INDEX NAME)

L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

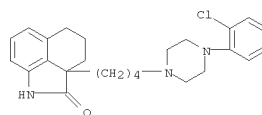


● HCl

RN 201608-55-1 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-[3-
(trifluoromethyl)phenyl]-1-piperazinyl]butyl]- (CA INDEX NAME)



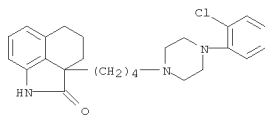
RN 201608-56-2 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a-[4-[4-(2-chlorophenyl)-1-piperazinyl]butyl]-
2a,3,4,5-tetrahydro-, hydrochloride (1:1) (CA INDEX NAME)



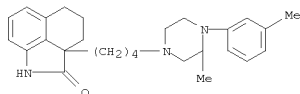
● HCl

RN 201608-57-3 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a-[4-[4-(2-chlorophenyl)-1-piperazinyl]butyl]-
2a,3,4,5-tetrahydro- (CA INDEX NAME)

L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

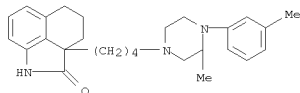


RN 201608-58-4 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[3-methyl-4-(3-
methylphenyl)-1-piperazinyl]butyl]-, hydrochloride (1:1) (CA INDEX NAME)



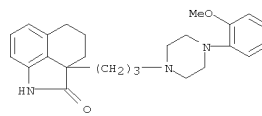
● HCl

RN 201608-59-5 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[3-methyl-4-(3-
methylphenyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



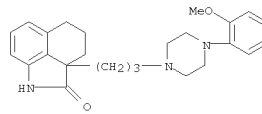
RN 201608-60-8 CAPLUS
CN Benz[cd]indol-2(1H)-one,
2a,3,4,5-tetrahydro-2a-[3-[4-(2-methoxyphenyl)-1-
piperazinyl]propyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

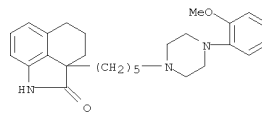


● HCl

RN 201608-61-9 CAPLUS
CN Benz[cd]indol-2(1H)-one,
2a,3,4,5-tetrahydro-2a-[3-[4-(2-methoxyphenyl)-1-
piperazinyl]propyl]- (CA INDEX NAME)



RN 201608-64-2 CAPLUS
CN Benz[cd]indol-2(1H)-one,
2a,3,4,5-tetrahydro-2a-[5-[4-(2-methoxyphenyl)-1-
piperazinyl]pentyl]-, hydrochloride (1:1) (CA INDEX NAME)

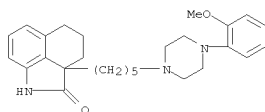


● HCl

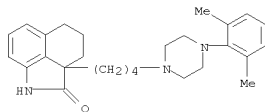
RN 201608-65-3 CAPLUS
CN Benz[cd]indol-2(1H)-one,
2a,3,4,5-tetrahydro-2a-[5-[4-(2-methoxyphenyl)-1-
piperazinyl]pentyl]- (CA INDEX NAME)

10590585.trn

L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

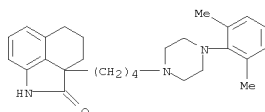


RN 201608-68-6 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a-[4-[4-(2,6-dimethylphenyl)-1-piperazinyl]butyl]-2a,3,4,5-tetrahydro-, hydrochloride (1:1) (CA INDEX NAME)



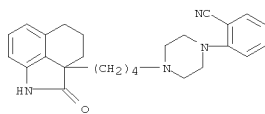
● HCl

RN 201608-69-7 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a-[4-[4-(2,6-dimethylphenyl)-1-piperazinyl]butyl]-2a,3,4,5-tetrahydro- (CA INDEX NAME)



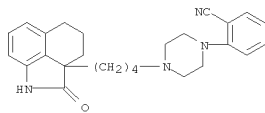
RN 201608-70-0 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-methoxyphenyl)-1-piperidinyl]butyl]- (CA INDEX NAME)

L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

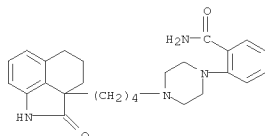


● HCl

RN 201608-78-8 CAPLUS
CN Benzonitrile, 2-[4-[4-(1,2,4,5-tetrahydro-2-oxobenz[cd]indol-2a(3H)-yl)butyl]-1-piperazinyl]- (CA INDEX NAME)

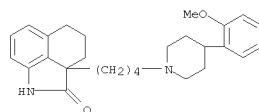


RN 201608-79-9 CAPLUS
CN Benzanide, 2-[4-[4-(1,2,4,5-tetrahydro-2-oxobenz[cd]indol-2a(3H)-yl)butyl]-1-piperazinyl]- (CA INDEX NAME)

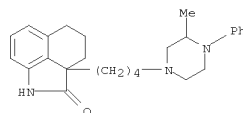


RN 201608-80-2 CAPLUS
CN Benzanide, 2-[4-[4-(1,2,4,5-tetrahydro-2-oxobenz[cd]indol-2a(3H)-yl)butyl]-1-piperazinyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

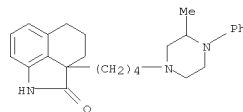


RN 201608-75-5 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(3-methyl-4-phenyl-1-piperazinyl)butyl]-, hydrochloride (1:1) (CA INDEX NAME)



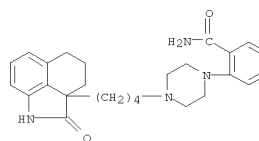
● HCl

RN 201608-76-6 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(3-methyl-4-phenyl-1-piperazinyl)butyl]- (CA INDEX NAME)



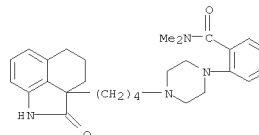
RN 201608-77-7 CAPLUS
CN Benzonitrile, 2-[4-[4-(1,2,4,5-tetrahydro-2-oxobenz[cd]indol-2a(3H)-yl)butyl]-1-piperazinyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

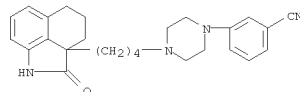


● HCl

RN 201608-81-3 CAPLUS
CN Benzanide, N,N-dimethyl-2-[4-[4-(1,2,4,5-tetrahydro-2-oxobenz[cd]indol-2a(3H)-yl)butyl]-1-piperazinyl]- (CA INDEX NAME)



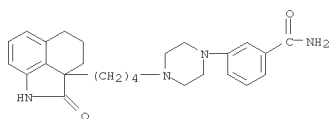
RN 201608-82-4 CAPLUS
CN Benzonitrile, 3-[4-[4-(1,2,4,5-tetrahydro-2-oxobenz[cd]indol-2a(3H)-yl)butyl]-1-piperazinyl]- (CA INDEX NAME)



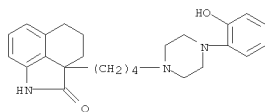
RN 201608-83-5 CAPLUS
CN Benzanide, 3-[4-[4-(1,2,4,5-tetrahydro-2-oxobenz[cd]indol-2a(3H)-yl)butyl]-1-piperazinyl]- (CA INDEX NAME)

10590585.trn

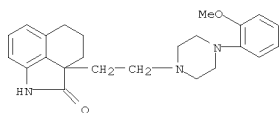
L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 201608-84-6 CAPLUS
CN Benz[cd]indol-2(1H)-one,
2a,3,4,5-tetrahydro-2a-[4-(2-hydroxyphenyl)-1-
piperazinyl]butyl]- (CA INDEX NAME)



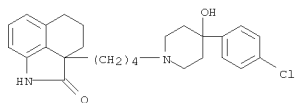
RN 201608-85-7 CAPLUS
CN Benz[cd]indol-2(1H)-one,
2a,3,4,5-tetrahydro-2a-[2-[4-(2-methoxyphenyl)-1-
piperazinyl]ethyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

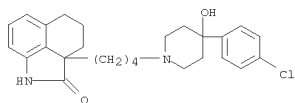
RN 201608-86-8 CAPLUS
CN Benz[cd]indol-2(1H)-one,
2a,3,4,5-tetrahydro-2a-[2-[4-(2-methoxyphenyl)-1-
piperazinyl]ethyl]- (CA INDEX NAME)

L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

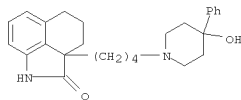


● HCl

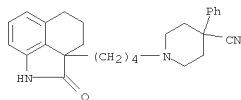
RN 201608-90-4 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a-[4-[4-(4-chlorophenyl)-4-hydroxy-1-
piperidinyl]butyl]-2a,3,4,5-tetrahydro- (CA INDEX NAME)



RN 201608-91-5 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-hydroxy-4-phenyl-1-
piperidinyl)butyl]- (CA INDEX NAME)

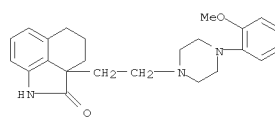


RN 201608-92-6 CAPLUS
CN 4-Piperidinecarbonitrile, 4-phenyl-1-[4-(1,2,4,5-tetrahydro-2-
oxobenz[cd]indol-2a(3H)-yl)butyl]-, hydrochloride (1:1) (CA INDEX NAME)

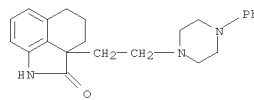


● HCl

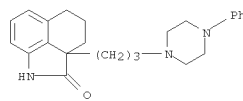
L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 201608-87-9 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[2-(4-phenyl-1-
piperazinyl)ethyl]- (CA INDEX NAME)



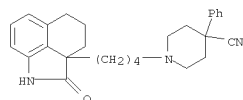
RN 201608-88-0 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[3-(4-phenyl-1-
piperazinyl)propyl]- (CA INDEX NAME)



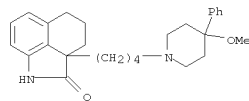
RN 201608-89-1 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a-[4-[4-(4-chlorophenyl)-4-hydroxy-1-
piperidinyl]butyl]-2a,3,4,5-tetrahydro-, hydrochloride (1:1) (CA INDEX
NAME)

L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

RN 201608-93-7 CAPLUS
CN 4-Piperidinecarbonitrile, 4-phenyl-1-[4-(1,2,4,5-tetrahydro-2-
oxobenz[cd]indol-2a(3H)-yl)butyl]- (CA INDEX NAME)

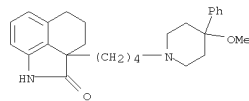


RN 201608-94-8 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-methoxy-4-phenyl-1-
piperidinyl)butyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

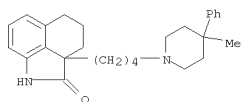
RN 201608-95-9 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-methoxy-4-phenyl-1-
piperidinyl)butyl]- (CA INDEX NAME)



RN 201608-96-0 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-methyl-4-phenyl-1-
piperidinyl)butyl]-, hydrochloride (1:1) (CA INDEX NAME)

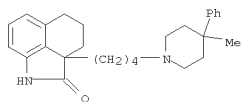
10590585.trn

L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

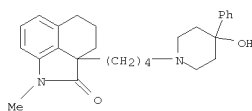


● HCl

RN 201608-97-1 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-methyl-4-phenyl-1-piperidinyl)butyl]- (CA INDEX NAME)

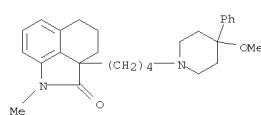


RN 201608-98-2 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-hydroxy-4-phenyl-1-piperidinyl)butyl]-1-methyl- (CA INDEX NAME)

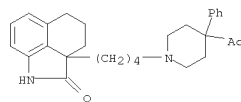


RN 201608-99-3 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-methoxy-4-phenyl-1-piperidinyl)butyl]-1-methyl- (CA INDEX NAME)

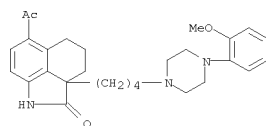
L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 201609-01-0 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a-[4-(4-acetyl-4-phenyl-1-piperidinyl)butyl]-2a,3,4,5-tetrahydro- (CA INDEX NAME)

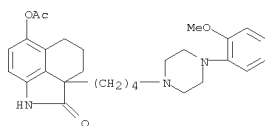


RN 201609-03-2 CAPLUS
CN Benz[cd]indol-2(1H)-one, 6-acetyl-2a,3,4,5-tetrahydro-2a-[4-(4-(2-methoxyphenyl)-1-piperazinyl)butyl]- (CA INDEX NAME)

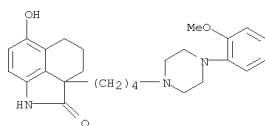


RN 201609-06-5 CAPLUS
CN Benz[cd]indol-2-one, 6-(acetyloxy)-1,2,2a,3,4,5-hexahydro-2a-[4-(4-(2-methoxyphenyl)-1-piperazinyl)butyl]- (CA INDEX NAME)

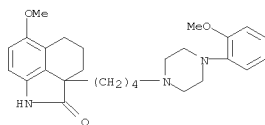
L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 201609-07-6 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-6-hydroxy-2a-[4-(4-(2-methoxyphenyl)-1-piperazinyl)butyl]- (CA INDEX NAME)

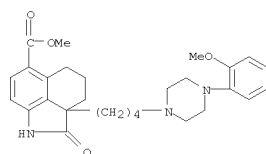


RN 201609-11-2 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-6-methoxy-2a-[4-(4-(2-methoxyphenyl)-1-piperazinyl)butyl]- (CA INDEX NAME)

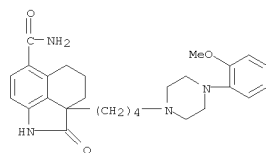


RN 201609-14-5 CAPLUS
CN Benz[cd]indole-6-carboxylic acid, 1,2,2a,3,4,5-hexahydro-2a-[4-(4-(2-methoxyphenyl)-1-piperazinyl)butyl]-2-oxo-, methyl ester (CA INDEX NAME)

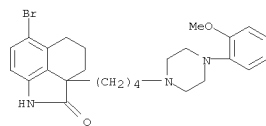
L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 201609-16-7 CAPLUS
CN Benz[cd]indole-6-carboxamide, 1,2,2a,3,4,5-hexahydro-2a-[4-(4-(2-methoxyphenyl)-1-piperazinyl)butyl]-2-oxo- (CA INDEX NAME)



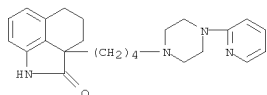
RN 201609-18-9 CAPLUS
CN Benz[cd]indol-2(1H)-one, 6-bromo-2a,3,4,5-tetrahydro-2a-[4-(4-(2-methoxyphenyl)-1-piperazinyl)butyl]- (CA INDEX NAME)



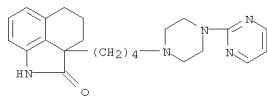
RN 201609-20-3 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-(4-(2-pyridinyl)-1-piperazinyl)butyl]- (CA INDEX NAME)

10590585.trn

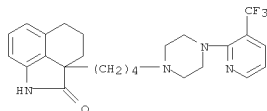
L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



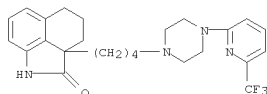
RN 201609-21-4 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-(2-pyrimidinyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



RN 201609-22-5 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-[3-(trifluoromethyl)-2-pyridinyl]-1-piperazinyl]butyl]- (CA INDEX NAME)



RN 201609-23-6 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-[6-(trifluoromethyl)-2-pyridinyl]-1-piperazinyl]butyl]- (CA INDEX NAME)

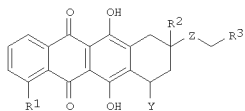


L25 ANSWER 60 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1998:42309 Document No. 128:1019570 Original Reference No.
128:19973a,19976a

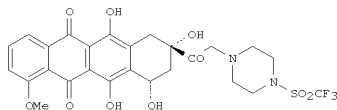
Preparation of fluoro-substituted anthracyclines for use as [19F]-MRI probes for monitoring amyloidotic diseases. Bandiera, Tiziano; Fancelli, Daniele; Caruso, Michele; Lanssen, Jacqueline; Suarato, Antonio (Pharmacia & Upjohn S.P.A., Italy). PCT Int. Appl. WO 9749433 A1 19971231, 42 pp. DESIGNATED STATES: W: AU, BG, BR, CA, CN, CZ, HU, IL, JP, KR, MX, NO,

NZ, PL, SG, SI, UA, US, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXKD2. APPLICATION: WO 1997-EP3234 19970618. PRIORITY: GB 1996-13433 19960626.

GI



I



II

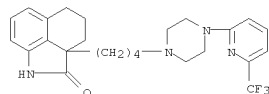
AB Fluorine substituted anthracyclines I [R1 = H, OH, halogen, alkoxy, amino, alkylsulfonyloxy, arylsulfonyloxy; R2 = H, OH; R3 = H, OH, amino, saccharide, heterocyclyl such as morpholino or piperazino; Y = H, OH, alkoxy, amino, heterocyclyl; Z = CO, CH(OH), CH2] were prepared for use

as NMR imaging probes which are useful in the diagnosis of amyloidosis. Thus, anthracycline II was prepared starting from 14-bromodaunomycinone, piperazine and triflic acid anhydride and gave an EC50 value of 8.16 ± 1.32 μM when tested for binding with fibrils from Aβ(25-35) peptide as compared with 52.04 ± 10.66 μM for iododoxorubicin.

IT 201344-98-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of fluoro-substituted anthracyclines for use as [19F]-MRI probes for monitoring amyloidotic diseases)

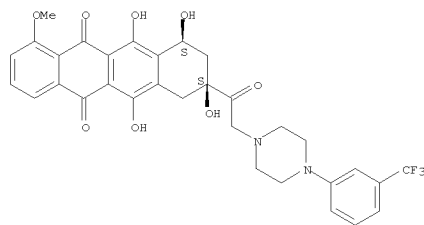
RN 201344-98-1 CAPLUS
CN 5,12-Naphthacenedione, 7,8,9,10-tetrahydro-6,8,10,11-tetrahydroxy-1-methoxy-8-[2-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]acetyl]-, (8S,10S)- (CA INDEX NAME)

L25 ANSWER 59 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
RN 201609-24-7 CAPLUS
CN Benz[cd]indol-2(1H)-one, 2a,3,4,5-tetrahydro-2a-[4-[4-[6-(trifluoromethyl)-2-pyridinyl]-1-piperazinyl]butyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

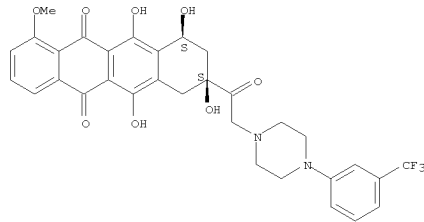
L25 ANSWER 60 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
Absolute stereochemistry.



IT 201344-89-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of fluoro-substituted anthracyclines for use as [19F]-MRI probes for monitoring amyloidotic diseases)

RN 201344-89-0 CAPLUS
CN 5,12-Naphthacenedione, 7,8,9,10-tetrahydro-6,8,10,11-tetrahydroxy-1-methoxy-8-[2-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]acetyl]-, hydrochloride (1:1), (8S,10S)- (CA INDEX NAME)

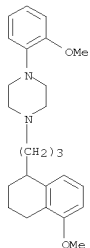
Absolute stereochemistry.



● HCl

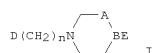
10590585.trn

L25 ANSWER 61 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1997:390206 Document No. 127:90128 Original Reference No. 127:17157a,17160a
 1-(2-Methoxyphenyl)-4-alkylpiperazines: effect of the N-4 substituent on
 the affinity and selectivity for dopamine D4 receptor. Perrone, Roberto;
 Berardi, Francesco; Colabufio, Nicola A.; Leopoldo, Marcello; Tortorella,
 Vincenzo (Dip. Farm.-Chim., Bari, 70126, Italy). Bioorganic & Medicinal
 Chemistry Letters, 7(10), 1327-1330 (English) 1997. CODEN: BMCLE8.
 ISSN:
 0960-894X. Publisher: Elsevier.
 AB Binding data on dopaminergic D2 and D4 and adrenergic $\alpha 1$ receptors
 of nine 1-(2-methoxyphenyl)piperazine derivs. are reported. The
 benzamide
 derivative 11 and ketone 12 displayed the highest affinity for human
 cloned D4
 receptor (K_i = 1.3 nM and 1.7 nM, resp.). The former showed to be also
 selective vs. D2 and $\alpha 1$ receptors.
 IT 154744-87-3P 178452-24-9P
 RI: BAC (Biological activity or effector, except adverse); BSU
 (Biological
 study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL
 (Biological study); PREP (Preparation)
 (1-(2-methoxyphenyl)piperazine derivs binding to dopaminergic D2 and
 D4
 and adrenergic $\alpha 1$ receptors)
 RN 154744-87-3 CAPLUS
 CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-
 naphthalenyl)propyl]- (CA INDEX NAME)



RN 178452-24-9 CAPLUS
 CN Piperazine, 1-(2-methoxyphenyl)-4-[4-(1,2,3,4-tetrahydro-5-methoxy-1-
 naphthalenyl)butyl]- (CA INDEX NAME)

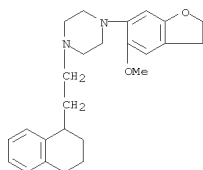
L25 ANSWER 62 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1997:67168 Document No. 126:893960 Original Reference No. 126:17267a
 Preparation of piperazine, piperidine, and 1,2,5,6-tetrahydropyridine
 derivatives and pharmaceutical compositions containing them. Peglioni,
 Jean-Louis; Dessinges, Aimee; Goument, Bertrand; Millan, Mark;
 Newman-Tancredi, Adrian; Gobert, Alain (Adir Et Compagnie, Fr.). Eur.
 Pat. Appl. EP 745598 A1 19961204, 29 pp. DESIGNATED STATES: R: AT, BE,
 CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE. (French).
 CODEN: EPXKDW. APPLICATION: EP 1996-401156 19960530. PRIORITY: FR
 1995-6436 19950531.
 GI



AB I (AB = CH2CH, CH:C, CH2N; n = 0-6; D = bicyclic ring system; E =
 heterocyclyl) were prepared E.g., coupling of 2-indancarboxylic acid
 with
 4-(2,3-dihydrobenzo-1,4-dioxin-6-yl)piperazine in the presence of
 carbonyldiimidazole gave an intermediate amide, which was reduced to give
 the dihydrochloride of 4-(2,3-dihydrobenzo-1,4-dioxin-6-yl)-1-(indan-2-
 ylmethyl)piperazine (II). The affinity of II for dopaminergic D4
 receptors was determined
 IT 185514-59-4P 185514-80-1P 185514-82-3P
 185515-26-8P
 RI: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and pharmacol. study of piperazine, piperidine, and
 1,2,5,6-tetrahydropyridine derivs.)
 RN 185514-59-4 CAPLUS
 CN Piperazine, 1-(2,3-dihydro-5-methoxy-6-benzofuranyl)-4-[2-(1,2,3,4-
 tetrahydro-1-naphthalenyl)ethyl]-, (2E)-2-butenedioate (1:1) (CA INDEX
 NAME)

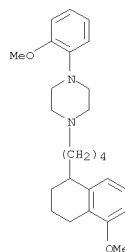
CM 1

CRN 185514-58-3
 CMF C25 H32 N2 O2



CM 2

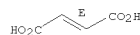
L25 ANSWER 61 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



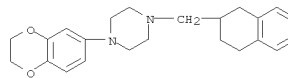
L25 ANSWER 62 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CRN 110-17-8
 CMF C4 H4 O4

Double bond geometry as shown.



RN 185514-80-1 CAPLUS
 CN Piperazine,
 1-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[(1,2,3,4-tetrahydro-2-
 naphthalenyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

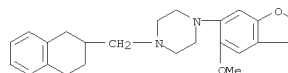


● HCl

RN 185514-82-3 CAPLUS
 CN Piperazine, 1-(2,3-dihydro-5-methoxy-6-benzofuranyl)-4-[(1,2,3,4-
 tetrahydro-2-naphthalenyl)methyl]-, (2E)-2-butenedioate (1:1) (CA INDEX
 NAME)

CM 1

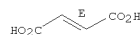
CRN 185514-81-2
 CMF C24 H30 N2 O2



CM 2

CRN 110-17-8
 CMF C4 H4 O4

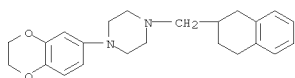
Double bond geometry as shown.



RN 185515-26-8 CAPLUS
 CN Piperazine,
 1-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[(1,2,3,4-tetrahydro-2-
 naphthalenyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

10590585.trn

L25 ANSWER 62 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
naphthalenyl)methyl]- (CA INDEX NAME)



L25 ANSWER 63 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1996;681311 Document No. 126;14313 Original Reference No. 126;2869a,2872a
Structure-Activity Relationship Studies on the 5-HT1A Receptor Affinity
of

1-Phenyl-4-[(α - or β -tetralinyl)alkyl]piperazines. 4.
Perrone, Roberto; Berardi, Francesco; Colabufo, Nicola A.; Leopoldo,
Marcello; Tortorella, Vincenzo; Fornaretto, Maria Gioia; Caccia, Carla;
McArthur, Robert A. (Dipartimento Farmaco-chimico, Universita di Bari,
Bari, 70126, Italy). Journal of Medicinal Chemistry, 39(25), 4928-4934
(English) 1996. CODEN: JMCMAR. ISSN: 0022-2623. Publisher: American
Chemical Society.

AB The synthesis of 1-phenylpiperazines, linked in the α or β
position of the tetralin moiety on the terminal part of the N-4 alkyl
chain, and their radioligand binding affinities for 5-HT1A, 5-HT2A, D-1,
D-2, α 1, and α 2 receptors along with SAR studies on the 5-HT1A
receptor are reported. Several changes have been carried out on previous
structures of type 2, by inserting the alkyl chain with variable length

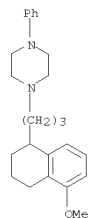
in
the α or β position of the tetralin moiety and by changing the
position of the methoxy group on the aromatic ring of the tetralin
nucleus.

The highest affinity (IC50 = 0.50 nM) and selectivity for the 5-HT1A
receptor were showed by the 1-phenylpiperazine derivative with a
three-membered alkyl chain bearing a 1-(5-methoxytetralin-1-yl) ring in
the α position.

IT 154744-86-2 154744-87-3 154744-88-4
184346-64-3
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP
(Properties); BIOL (Biological study); PROC (Process)
(preparation and structure-activity relationship studies on serotonin

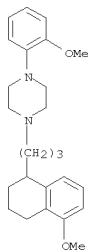
S1A receptor affinity of phenyl[α - or
 β -tetralinyl]alkyl]piperazines)

RN 154744-86-2 CAPLUS
CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-
naphthalenyl)propyl]- (CA INDEX NAME)

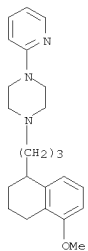


RN 154744-87-3 CAPLUS

L25 ANSWER 63 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-
naphthalenyl)propyl]- (CA INDEX NAME)

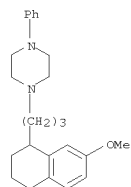


RN 154744-88-4 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-
naphthalenyl)propyl]- (CA INDEX NAME)



RN 184346-64-3 CAPLUS
CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-
naphthalenyl)propyl]- (CA INDEX NAME)

L25 ANSWER 63 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

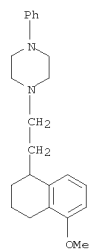


IT 184347-24-8P 184347-26-0P 184347-28-2P
184347-33-9P 184347-43-1P 184347-45-3P
184347-47-5P

RL: BPR (Biological process); BSU (Biological study, unclassified); PRP
(Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or
reagent)

(preparation and structure-activity relationship studies on serotonin
S1A receptor affinity of phenyl[α - or
 β -tetralinyl]alkyl]piperazines)

RN 184347-24-8 CAPLUS
CN Piperazine, 1-phenyl-4-[2-(1,2,3,4-tetrahydro-5-methoxy-1-
naphthalenyl)ethyl]-, hydrochloride (1:2) (CA INDEX NAME)

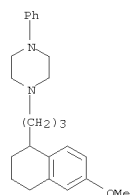


● 2 HCl

RN 184347-26-0 CAPLUS
CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-6-methoxy-1-
naphthalenyl)propyl]-, hydrochloride (1:2) (CA INDEX NAME)

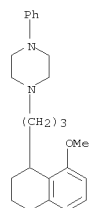
10590585.trn

L25 ANSWER 63 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



●2 HCl

RN 184347-28-2 CAPLUS
CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-8-methoxy-1-naphthalenyl)propyl]-, hydrochloride (1:2) (CA INDEX NAME)

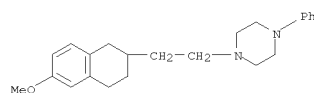


●2 HCl

RN 184347-33-9 CAPLUS
CN Piperazine, 1-phenyl-4-[4-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)butyl]-, hydrochloride (1:2) (CA INDEX NAME)

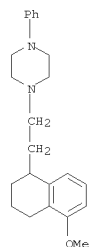
L25 ANSWER 63 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

RN 184347-47-5 CAPLUS
CN Piperazine, 1-phenyl-4-[2-(1,2,3,4-tetrahydro-6-methoxy-2-naphthalenyl)ethyl]-, hydrochloride (1:2) (CA INDEX NAME)



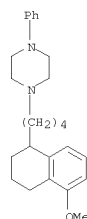
●2 HCl

IT 184346-68-7P 184346-70-1P 184346-72-3P
184346-77-8P 184346-86-9P 184346-89-2P
184346-91-6P
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
S1A (preparation and structure-activity relationship studies on serotonin receptor affinity of phenyl[α - or β -tetralinyl]alkyl]piperazines)
RN 184346-68-7 CAPLUS
CN Piperazine, 1-phenyl-4-[2-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)ethyl]- (CA INDEX NAME)



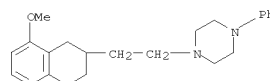
RN 184346-70-1 CAPLUS
CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-6-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)

L25 ANSWER 63 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



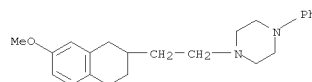
●2 HCl

RN 184347-43-1 CAPLUS
CN Piperazine, 1-phenyl-4-[2-(1,2,3,4-tetrahydro-8-methoxy-2-naphthalenyl)ethyl]-, hydrochloride (1:2) (CA INDEX NAME)



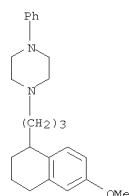
●2 HCl

RN 184347-45-3 CAPLUS
CN Piperazine, 1-phenyl-4-[2-(1,2,3,4-tetrahydro-7-methoxy-2-naphthalenyl)ethyl]-, hydrochloride (1:2) (CA INDEX NAME)

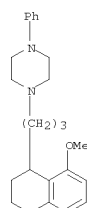


●2 HCl

L25 ANSWER 63 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



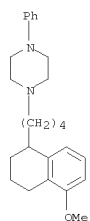
RN 184346-72-3 CAPLUS
CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-8-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)



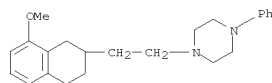
RN 184346-77-8 CAPLUS
CN Piperazine, 1-phenyl-4-[4-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)butyl]- (CA INDEX NAME)

10590585.trn

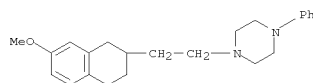
L25 ANSWER 63 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 184346-86-9 CAPLUS
CN Piperazine, 1-phenyl-4-[2-(1,2,3,4-tetrahydro-8-methoxy-2-naphthalenyl)ethyl]- (CA INDEX NAME)



RN 184346-89-2 CAPLUS
CN Piperazine, 1-phenyl-4-[2-(1,2,3,4-tetrahydro-7-methoxy-2-naphthalenyl)ethyl]- (CA INDEX NAME)



RN 184346-91-6 CAPLUS
CN Piperazine, 1-phenyl-4-[2-(1,2,3,4-tetrahydro-6-methoxy-2-naphthalenyl)ethyl]- (CA INDEX NAME)

L25 ANSWER 64 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1996:522872 Document No. 125:211514 Original Reference No. 125:39263a,39266a

Dopamine and serotonin receptor antagonists. Synthesis of aminoalkyl cyclanones as atypical antipsychotics. Ravina Rubira, E. (Departamento de Química Orgánica, Facultad de Farmacia, Santiago de Compostela, 15706, Spain). *Ars Pharmaceutica*, 36(3), 337-376 (Spanish) 1995. CODEN: APHRAN.

ISSN: 0004-2927. Publisher: Universidad de Granada, Facultad de Farmacia.

AB A review with 48 refs. A series of 3-aminomethyl tetralones and 2-aminoethyl cycloalkanones carrying o-methoxy phenylpiperazine, p-fluoro butyrophene and p-fluorobenzoyl piperidine fragments have been prepared. The new compds. have been evaluated as potential antipsychotic agents in receptor binding assays for dopamine D1 and D2 receptors and 5-HT2A serotonin receptors and in functional and behavioral screens. The ratios of pKi's for 5-HT2A/D2 receptors may be useful for rapid screening of new compds. and its potential induction of extrapyramidal symptoms (ratio values > 1.12 are predictive of an atypical antipsychotic profile). With the exception of QF 0100B, QF 0102B and QF 0309B, the new compds. had a ratio value in the range 1.08-1.20, while haloperidol showed a ratio of 0.93. In the catalepsy test (predictive test for induction of extrapyramidal symptoms) the values obtained were in accordance with atypical antipsychotic drug profiles. Likewise, a few 2-methyl-3-ethyl-5-aminomethyl-4-oxo-4, 5, 6, 7-tetrahydroindoles (QF 0400B, QF 0402B, QF 0403B, QF 0404B) analogous of neuroleptic molindone receptors. Their affinities for D2 and 5-HT2A receptors are lower than haloperidol and comparable to those of molindone.

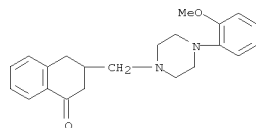
IT 133496-60-3P

RL: BAC (Biological activity or effector, except adverse); BSU

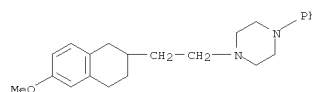
(Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (dopamine and serotonin receptor antagonists: synthesis of aminoalkyl cyclanones as atypical antipsychotics)

RN 133496-60-3 CAPLUS

CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)

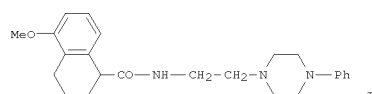


L25 ANSWER 63 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



L25 ANSWER 65 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1996:422514 Document No. 125:76102 Original Reference No. 125:14243a,14246a
1-Aryl-4-[(1-tetralinyl)alkyl]piperazines: alkylamido and alkylamino derivatives. Synthesis, 5-HT1A receptor affinity, and selectivity. 3. Perrone, Roberto; Berardi, Francesco; Leopoldo, Marcello; Tortorella, Vincenzo; Fornaretto, Maria Gioia; Caccia, Carla; McArthur, Robert A. (Dipartimento Farmaco-chimico, Università di Bari, Bari, 70126, Italy). *Journal of Medicinal Chemistry*, 39(16), 3195-3202 (English) 1996. CODEN: JMCMAR. ISSN: 0022-2623. Publisher: American Chemical Society.

GI



AB The synthesis and binding profile on 5-HT1A, 5-HT2, D-1, D-2, α1, and α2 receptors of the N-4 long-chain arylpiperazines 22-40 are reported, where an amino or amido function is inserted into the intermediate chain linked to the α position of the tetralin nucleus, as in I. Unlike the buspirone analogs, for the amido derivs. studied in this paper, the terminal amide function of long-chain piperazines is not important for 5-HT1A receptor affinity binding, and its removal yields high-affinity 5-HT1A receptor agents.

IT 154744-86-2 154744-87-3 154744-88-4

178452-24-9 RL: BAC (Biological activity or effector, except adverse); BPR

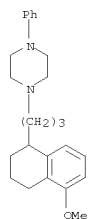
(Biological process); BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent) (preparation, 5-HT1A receptor affinity, and selectivity of 1-aryl-4-[(1-tetralinyl)alkyl]piperazine alkylamido and alkylamino derivs.)

RN 154744-86-2 CAPLUS

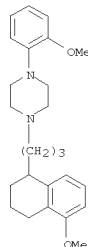
CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)

10590585.trn

L25 ANSWER 65 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

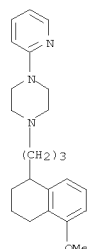


RN 154744-87-3 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[(3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl)-] (CA INDEX NAME)

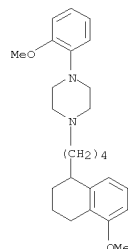


RN 154744-88-4 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[(3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl)-] (CA INDEX NAME)

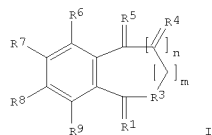
L25 ANSWER 65 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 178452-24-9 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[(4-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)butyl)-] (CA INDEX NAME)

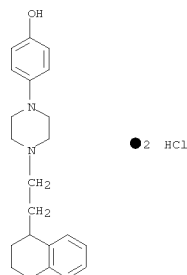


L25 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1995:951193 Document No. 124:88450 Original Reference No. 124:1873a,1876a
Preparation of heterocyclic compounds for the treatment of CNS and cardiovascular disorders. Ten Brink, Ruth E.; Ennis, Michael D.; Lin, Chiu-Hong; Lahti, Robert A.; Romero, Arthur G.; Sih, John C. (Upjohn Co., USA). PCT Int. Appl. WO 9518118 A1 19950706, 197 pp. DESIGNATED STATES: W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2.
APPLICATION: WO 1994-US13284 19941130. PRIORITY: US 1993-175218
19931228;
US 1994-279974 19940725.
GI

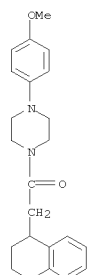


AB The title compds. (I; R1 = H, alkyl, etc.; R3 = O, S; R4 = H, alkyl, Ph, OH, etc.; R5 = H, alkyl, Ph, OH, alkoxy; R6-R9 = F, Cl, Br, I, H, etc.;
m,
n = 0, 1), useful as CNS (no data) and cardiovascular (no data) agents, are prepared. Thus, 1-(2-chloroethyl)isochroman was reacted with 1-(2-chlorophenyl)piperazine dihydrochloride, producing 1-(2-chlorophenyl)-4-[2-(isochroman-1-yl)ethyl]piperazine hydrochloride, m.p. 197-198°.
IT 170856-48-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent).
(preparation of heterocyclic compds. for the treatment of CNS and cardiovascular disorders)
RN 170856-48-1 CAPLUS
CN Phenol,
4-[4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-1-piperazinyl]-, hydrochloride (1:2) (CA INDEX NAME)

L25 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



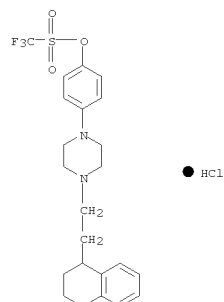
IT 170857-41-7P 170857-43-9P 170857-55-3P
170857-76-8P 170857-78-0P 170857-79-1P
170857-80-4P 170857-82-6P 170857-83-7P
170857-84-8P 170857-85-9P 170857-86-0P
170857-87-1P 170858-80-7P 170858-81-8P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic compds. for the treatment of CNS and cardiovascular disorders)
RN 170857-41-7 CAPLUS
CN Ethanone, 1-[4-(4-methoxyphenyl)-1-piperazinyl]-2-(1,2,3,4-tetrahydro-1-naphthalenyl)- (CA INDEX NAME)



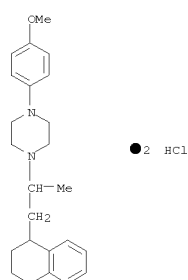
RN 170857-43-9 CAPLUS
CN Methanesulfonic acid, 1,1,1-trifluoro-,

10590585.trn

L25 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
4-[4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-1-piperazinyl]phenyl
ester, hydrochloride (1:1) (CA INDEX NAME)

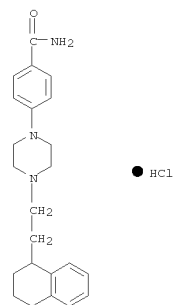


RN 170857-55-3 CAPLUS
CN Piperazine, 1-(4-methoxyphenyl)-4-[1-methyl-2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-, hydrochloride (1:2) (CA INDEX NAME)



RN 170857-76-8 CAPLUS
CN Benzamide, 4-[4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-1-

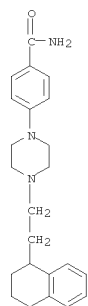
L25 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
piperazinyl]-, hydrochloride (1:1) (CA INDEX NAME)



RN 170857-78-0 CAPLUS
CN Benzamide, 4-[4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-1-piperazinyl]-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

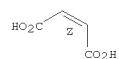
CM 1
CRN 170857-77-9
CMF C23 H29 N3 O

L25 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 2
CRN 110-16-7
CMF C4 H4 O4

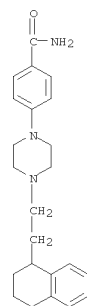
Double bond geometry as shown.



RN 170857-79-1 CAPLUS
CN Benzamide, 4-[4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-1-piperazinyl]-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

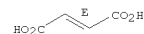
CM 1
CRN 170857-77-9
CMF C23 H29 N3 O

L25 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 2
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

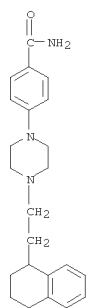


RN 170857-80-4 CAPLUS
CN Benzamide, 4-[4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-1-piperazinyl]-, methanesulfonate (1:1) (CA INDEX NAME)

CM 1
CRN 170857-77-9
CMF C23 H29 N3 O

10590585.trn

L25 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 2

CRN 75-75-2
CMF C H4 O3 S



RN 170857-82-6 CAPLUS
CN Benzenesulfonamide, 4-[4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-1-piperazinyl]-, (R)-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 170857-81-5
CMF C22 H29 N3 O2 S

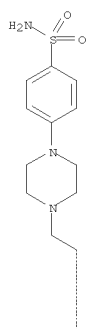
Absolute stereochemistry.

L25 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
1-piperazinyl]-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

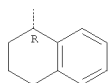
CM 1

CRN 170857-81-5
CMF C22 H29 N3 O2 S

Absolute stereochemistry.



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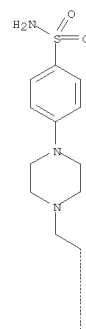
CM 2

CRN 110-16-7
CMF C4 H4 O4

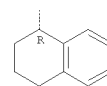
Double bond geometry as shown.

L25 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

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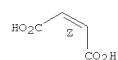
CM 2

CRN 75-75-2
CMF C H4 O3 S



RN 170857-83-7 CAPLUS
CN Benzenesulfonamide, 4-[4-[2-[(1R)-1,2,3,4-tetrahydro-1-naphthalenyl]ethyl]-1-piperazinyl]benzenesulfonamide (1:1) (9CI) (CA INDEX NAME)

L25 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



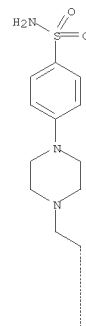
RN 170857-84-8 CAPLUS
CN Propanoic acid, 2-hydroxy-, compd. with (R)-4-[4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-1-piperazinyl]benzenesulfonamide (1:1) (9CI) (CA INDEX NAME)

CM 1

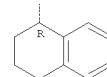
CRN 170857-81-5
CMF C22 H29 N3 O2 S

Absolute stereochemistry.

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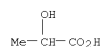


CM 2

10590585.trn

L25 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CRN 50-21-5
CMF C3 H6 O3



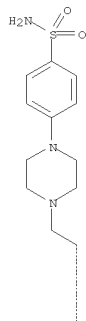
RN 170857-85-9 CAPLUS
CN Benzenesulfonamide, 4-[4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-1-piperazinyl]-, (R)-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

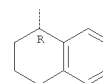
CRN 170857-81-5
CMF C22 H29 N3 O2 S

Absolute stereochemistry.

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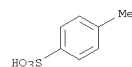


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CM 2

CRN 104-15-4
CMF C7 H8 O3 S



RN 170857-86-0 CAPLUS
CN Benzenesulfonamide, 4-[4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-1-piperazinyl]-, (R)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (9CI) (CA INDEX NAME)

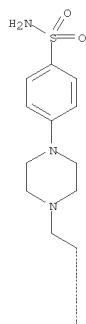
CM 1

CRN 170857-81-5
CMF C22 H29 N3 O2 S

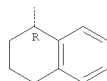
Absolute stereochemistry.

L25 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

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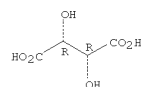
PAGE 2-A



CM 2

CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.



RN 170857-87-1 CAPLUS
CN Benzenesulfonamide, 4-[4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-1-piperazinyl]-, (R)-, 2-hydroxy-1,2,3-propanetricarboxylate (1:1) (9CI) (CA INDEX NAME)

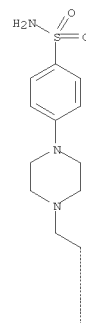
L25 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CM 1

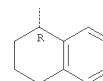
CRN 170857-81-5
CMF C22 H29 N3 O2 S

Absolute stereochemistry.

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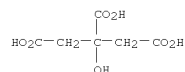


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CM 2

CRN 77-92-9
CMF C6 H8 O7



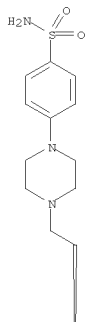
10590585.trn

L25 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

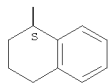
RN 170858-80-7 CAPLUS
CN Benzenesulfonamide, 4-[4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-1-piperazinyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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RN 170858-81-8 CAPLUS
CN Benzenesulfonamide, 4-[4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-1-piperazinyl]-, (S)-, monomethanesulfonate (9CI) (CA INDEX NAME)

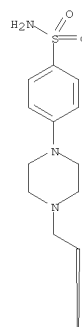
CM 1

CRN 170858-80-7
CMF C22 H29 N3 O2 S

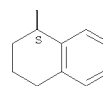
Absolute stereochemistry. Rotation (-).

L25 ANSWER 66 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

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PAGE 2-A



CM 2

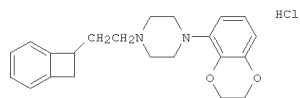
CRN 75-75-2
CMF C H4 O3 S



L25 ANSWER 67 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1995:790900 Document No. 124:1347420 Original Reference No.
124:24730h,24731a Characterization of Potent and Selective Antagonists

at Postsynaptic 5-HT1A Receptors in a Series of N4-Substituted Arylpiperazines. Peglioni, Jean-Louis; Canton, Herve; Bervoets, Karin; Audinot, Valerie; Brocco, Mauricette; Gobert, Alain; Le Marouille-Girardon, Sylvie; Millan, Mark J. (Institut de Recherches Servier, Suresnes, 92150, Fr.). Journal of Medicinal Chemistry, 38(20), 4044-55 (English) 1995. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 124:134742. Publisher: American Chemical Society.

GI



AB Benzocycloalkyl and benzocycloalkenyl moieties linked, directly or via an alkyl chain, to oxygen-bearing heteroarylpiperazines were synthesized, in an attempt to obtain potent and selective antagonists at postsynaptic 5-HT1A receptors. From the numerous arylpiperazines described in the literature, 1-(2,3-dihydro-1,4-benzodioxin-5-yl)piperazine was chosen as

a model of an arylpiperazine in view of its selectivity for 5-HT1A receptors

vs. α 1-, α 2-, and β -adrenergic receptors, as well as dopamine D1 and D2 receptors. Two other closely-related arylpiperazines, 1-(1,5-benzodioxepin-6-yl)piperazine and 1-(benzofuran-7-yl)piperazine, were also examined in this study. All compds. showed high affinity at 5-HT1A sites ($8.10 \leq pK_{is} < 9.35$), and the majority behaved as antagonists in vivo in blocking the hypothermia induced by the 5-HT1A agonist 8-OH-DPAT in the absence of a marked effect alone at equivalent doses.

An in vivo evaluation of dopamine D2 receptor antagonist properties revealed that the majority of compds. was devoid of activity at this site,

in marked contrast to BMY 7378 which displayed virtually no selectivity for 5-HT1A vs. dopamine D2 receptors. Moreover, six compds. of the present series, including I, showed >10-fold selectivity in vitro for 5-HT1A vs. α 1-adrenergic receptors. I displayed an optimal compromise between potency ($pK_i = 8.75$), marked antagonist activity, and selectivity toward α 1-adrenergic (81-fold) and dopamine D2 195-fold receptors. These characteristics clearly distinguish I from previously-reported ligands such as the postsynaptic 5-HT1A antagonist

BMY 7378 and the weak partial agonist NAN 190 which, in contrast to the compds. of this series, belong to the well-exemplified class of imido derivs. of (o-methoxyphenyl)piperazines. The availability of I (S 15535) should facilitate the further elucidation of the functional role and potential therapeutic significance of 5-HT1A receptors.

IT 168329-98-4F

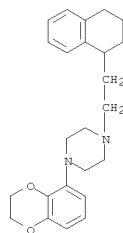
L25 ANSWER 67 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
RL: BAC (Biological activity or effector, except adverse); BSU

(Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(potent and selective antagonists at postsynaptic 5-HT1A receptors in

a series of N4-substituted arylpiperazines)

RN 168329-98-4 CAPLUS

CN Piperazine,
1-(2,3-dihydro-1,4-benzodioxin-5-yl)-4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

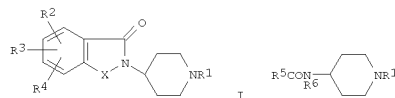


● HCl

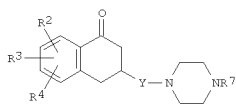
10590585.trn

L25 ANSWER 68 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1995:568500 Document No. 123:1695160 Original Reference No.
 123:30259a,30262a Preparation of acylaminopiperidines and piperazines as
 inhibitors of microsomal triglyceride transfer protein.. Wetterau, John
 R., II; Sharp, Daru Young; Gregg, Richard E.; Biller, Scott A.; Dickson,
 John K.; Lawrence, Michael R.; Lawson, John E.; Holava, Henry M.;
 Partyka, Richard A. (Bristol-Myers Squibb Co., USA). Eur. Pat. Appl. EP 643057 A1
 19950315, 134 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB,
 GR, IE, IT, LI, LU, MC, NL, PT, SE. (English). CODEN: EPXKDW.
 APPLICATION: EP 1994-113800 19940902. PRIORITY: US 1993-117362 19930903;
 US 1992-847503 19920306.

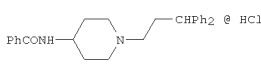
GI



II



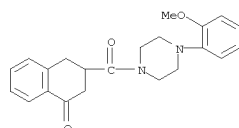
III



IV

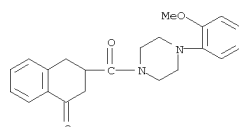
AB Title compds. [I-III; X = CHR8, CHR9CHR10, CR9:CR10; R8-R10 = H, alkyl,
 alkenyl, alkynyl, aryl, aralkyl, heteroaryl, heteroarylalkyl, cycloalkyl,
 cycloalkylalkyl; Y = (CH2)m, CO; m = 2, 3; R1 = (substituted) alkyl,
 alkenyl, alkynyl, aryl, heteroaryl, aralkyl, diarylalkyl, diarylalkenyl,
 diarylalkynyl, diarylalkylalkyl, heteroarylalkyl, cycloalkyl,
 cycloalkylalkyl, etc.; R2-R4 = H, halo, alkyl, haloalkyl, alkenyl,
 alkoxy,
 aryloxy, aryl, arylalkyl, alkylthio, arylthio, cycloalkyl,
 cycloalkylalkyl, heteroaryl, heteroarylalkyl, OH, haloalkyl; R5 =
 (substituted) alkyl, alkenyl, alkynyl, aryl, heteroaryl, aralkyl,
 heteroarylalkyl, cycloalkyl, cycloalkylalkyl, polycycloalkyl,
 cycloalkenyl, cycloalkenylalkyl, heteroarylcarbonyl, etc.; R6 = H, alkyl,
 alkenyl; R7 = alkyl, aryl, aralkyl, oxoalkyl, aryloxoalkyl], were
 prepared

L25 ANSWER 68 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

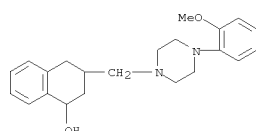


● HCl

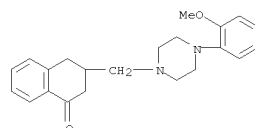
RN 163266-62-4 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[[4-(2-methoxyphenyl)-1-
 piperazinyl]carbonyl]- (CA INDEX NAME)



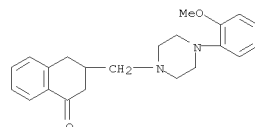
IT 163268-03-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of acylaminopiperidines and piperazines as inhibitors of
 microsomal triglyceride transfer protein)
 RN 163268-03-9 CAPLUS
 CN 1-Naphthalenol, 1,2,3,4-tetrahydro-3-[[4-(2-methoxyphenyl)-1-
 piperazinyl]methyl]- (CA INDEX NAME)



L25 ANSWER 68 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 as inhibitors of microsomal triglyceride transfer protein. Thus, tert-Bu
 4-piperidinylocarbamate (prepn. given) and 3,3-diphenyl-1-propanol
 tosylate
 (prepn. given) were stirred with K2CO3 in Me2CHOH overnight to give 76%
 tert-Bu [1-(3,3-diphenylpropyl)-4-piperidinylocarbamate. This was
 deprotected with 4N HCl in dioxane and the product was treated with
 PhCOCl
 and Et3N in CH2Cl2 to give title compd. (IV).
 IT 133496-60-3P 133496-73-8P 163266-60-2P
 163266-62-4P
 RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of acylaminopiperidines and piperazines as inhibitors of
 microsomal triglyceride transfer protein)
 RN 133496-60-3 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[[4-(2-methoxyphenyl)-1-
 piperazinyl]methyl]- (CA INDEX NAME)



RN 133496-73-8 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[[4-(2-methoxyphenyl)-1-
 piperazinyl]methyl]-, hydrochloride (1:2) (CA INDEX NAME)



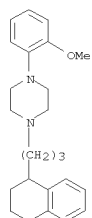
● 2 HCl

RN 163266-60-2 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[[4-(2-methoxyphenyl)-1-
 piperazinyl]carbonyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 69 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1995:413186 Document No. 122:204546 Original Reference No.
 122:37061a,37064a
 High Affinity and Selectivity on 5-HT1A Receptor of
 1-Aryl-4-[(1-tetralin)alkyl]piperazines. 2. Perrone, Roberto; Berardi,
 Francesco; Colabuso, Nicola A.; Leopoldo, Marcello; Tortorella, Vincenzo;
 Fiorentini, Francesco; Olgiati, Vincenzo; Ghiglieri, Alberto; Govoni,
 Stefano (Dipartimento Farmaco-chimico, Universita di Bari, Bari, 70126,
 Italy). Journal of Medicinal Chemistry, 38(6), 942-9 (English) 1995.
 CODEN: JMCMAR. ISSN: 0022-2623. Publisher: American Chemical Society.
 AB Several 4-alkyl-1-arylpiperazines that present a tetralin moiety on the
 terminal part of the side chain were synthesized in order to increase the
 selectivity on the 5-HT1A vs. D-2, α1, α, and other 5-HT
 receptors. Many changes have been effected on previous structures of
 type
 3 (1-aryl-4-[3-(1,2-dihydronaphthalen-4-yl)-n-propyl]piperazines).
 Several synthetic procedures were followed to obtain the final products,
 depending on the presence or absence of a double bond, as well as of a
 heteroatom on the side chain. In the first case versatile use of
 Grignard
 reaction was made, whereas in the second one usual synthetic ways were
 applied. Final compds. were evaluated for in vitro activity on dopamine
 D-1 and D-2, serotonin 5-HT1A, 5-HT1B, 5-HT1C, and 5-HT2, α1
 adrenergic, and α receptors by radioreceptor binding assay. For the
 2-MeO-Ph, 2-pyridyl, and unsubstituted Ph N-piperazine derivs., low IC50
 values (0.3 nM) on 5-HT1A receptors and high selectivity values were
 observed
 IT 161923-75-7P 161923-76-8P 161923-77-9P
 161923-78-0P 161923-79-1P 161923-85-9P
 161923-86-0P 161923-87-1P 161923-88-2P
 161923-89-3P 161923-90-6P
 RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)
 (high affinity and selectivity on 5-HT1A receptor of
 aryl[(tetralin)alkyl]piperazines)
 RN 161923-75-7 CAPLUS
 CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-1-
 naphthalenyl)propyl]-, hydrochloride (1:2) (CA INDEX NAME)

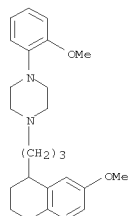
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L25 ANSWER 69 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● 2 HCl

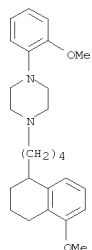
RN 161923-76-8 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

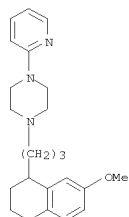
RN 161923-77-9 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]-, hydrochloride (1:2) (CA INDEX NAME)

L25 ANSWER 69 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● 2 HCl

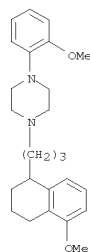
RN 161923-85-9 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]-, hydrochloride (1:3) (CA INDEX NAME)



● 3 HCl

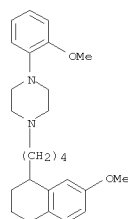
RN 161923-86-0 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]-, hydrochloride (1:2) (CA INDEX NAME)

L25 ANSWER 69 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● 2 HCl

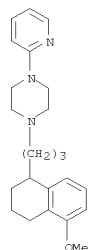
RN 161923-78-0 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[4-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)butyl]-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

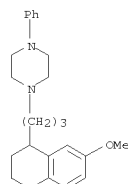
RN 161923-79-1 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[4-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)butyl]-, hydrochloride (1:2) (CA INDEX NAME)

L25 ANSWER 69 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● 2 HCl

RN 161923-87-1 CAPLUS
CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]-, hydrochloride (1:2) (CA INDEX NAME)

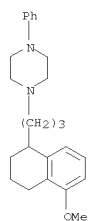


● 2 HCl

RN 161923-88-2 CAPLUS
CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]-, hydrochloride (1:2) (CA INDEX NAME)

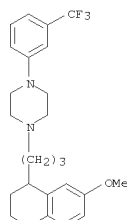
10590585.trn

L25 ANSWER 69 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● 2 HCl

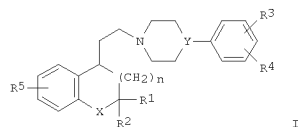
RN 161923-89-3 CAPLUS
CN Piperazine,
1-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 161923-90-6 CAPLUS
CN Piperazine,
1-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (2:3) (CA INDEX NAME)

L25 ANSWER 70 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1995:412830 Document No. 122:1876200 Original Reference No.
122:34375a,34378a Preparation of (benzocyclylethyl)aryl piperidines and -piperazines for treating arrhythmia and tachycardia.. Baumgarth, Manfred; Lues, Inge; Minck, Klaus-Otto; Beier, Norbert (Merck Patent GmbH, Germany). Ger. Offen. DE 4321366 A1 19950105, 10 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1993-4321366 19930626.
GI

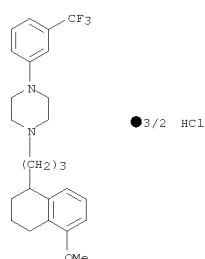


AB Title compds. [I; R1, R2 = H, alkyl; R3-R5 = H, halo, OH, alkoxy, alkanoyloxy, NO2, NR2, alkanoylamino, alkylsulfonylamino, cyano; R3R4 = O(CH2)mO; n = 0-2; X = O, CH2, NH, alkylimino, alkanoylimino; Y = CH, N; m = 1, 2], were prepared as for treating arrhythmia and tachycardia (no data).

Thus, 2-(6,7,8,9-tetrahydro-5H-benzocyclohepten-5-yl)ethyl bromide (preparation given), 4-(3,4-dimethoxyphenyl)piperidine hydrochloride, K2CO3, and KI were refluxed 3 h in MeCOEt to give 1-[2-(6,7,8,9-tetrahydro-5H-benzocyclohepten-5-yl)ethyl]-4-(3,4-dimethoxyphenyl)piperidine, which was converted to the fumarate.
IT 161525-18-4P 161525-24-2P 161525-26-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of (benzocyclylethyl)aryl piperidines and -piperazines for treating arrhythmia and tachycardia)

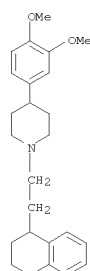
RN 161525-18-4 CAPLUS
CN Piperidine, 4-(3,4-dimethoxyphenyl)-1-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]- (CA INDEX NAME)

L25 ANSWER 69 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● 3/2 HCl

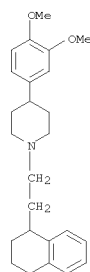
L25 ANSWER 70 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 161525-24-2 CAPLUS
CN Piperidine, 4-(3,4-dimethoxyphenyl)-1-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 161525-18-4
CMF C25 H33 N O2

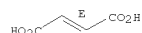


CM 2

CRN 110-17-8
CMF C4 H4 O4

10590585.trn

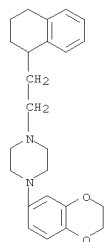
L25 ANSWER 70 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
Double bond geometry as shown.



RN 161525-26-4 CAPLUS
CN Piperazine,
1-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-(1,2,3,4-tetrahydro-
1-naphthalenyl)ethyl]-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 161525-25-3
CMP C24 H30 N2 O2



CM 2

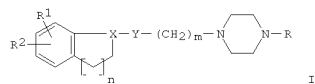
CRN 110-17-8
CMP C4 H4 O4

Double bond geometry as shown.

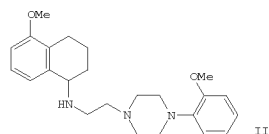


IT 161525-32-2 161525-33-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (benzocyclylethyl)aryl)piperidines and -piperazines for
treating arrhythmia and tachycardia)
RN 161525-32-2 CAPLUS
CN Ethanone,
1-[4-(3,4-dimethoxyphenyl)-1-piperidinyl]-2-(1,2,3,4-tetrahydro-

L25 ANSWER 71 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
1994:298643 Document No. 120:2986430 Original Reference No.
120:52637a, 52640a N-(hetero)aryl-N-[(hetero)tetralinalkyl]piperazine
having serotonergic, dopaminergic and adrenergic activity. Perrone,
Roberto; Berardi, Francesco; Fiorentini, Francesco; Govoni, Stefano;
Olgiaati, Vincenzo; Vanotti, Ermes; Gobetti, Marino; Tonon, Giancarlo
(Pierrel S.p.A., Italy). PCT Int. Appl. WO 9400441 A1 19940106, 72 pp.
DESIGNATED STATES: W: AU, BB, BG, BR, BY, CA, CZ, FI, HU, JP, KP, KR,
KZ,
LK, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US, VN; RW: AT, BE, BF,
BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML,
MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION:
WO 1993-EP1589 19930622. PRIORITY: IT 1992-MI1569 19920626.
GI



I



II

AB N-(aryl)-N'-(tetralinalkyl)piperazine having serotonergic, dopaminergic
and adrenergic activity, the processes for their preparation and relative
therapeutic compns. for the treatment of anxiety generated by depression,
for the treatment of schizophrenia, cerebral ischemia, opium like and
psycho stimulant substances abuse syndromes consciousness disorders such
as senile dementia, vigilance and memory disorders, Parkinson's and
Alzheimer's diseases and for the treatment of arterial hypertension.

More narrowly defined compds. are the N-(aryl)-N'-(tetralinalkyl)piperazines I
(R1, R2 = alkyl, alkoxy, etc.; R = aryl; XY = alkanediyl, etc.; n = 1,2;
m

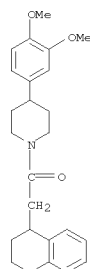
= 2,3). A specific compound is
1-(2-methoxyphenyl)-4-[2-[(5-methoxy-1,2,3,4-
tetrahydronaphthalen-1-yl)amino]ethyl]piperazine (II).

IT 154744-84-0P 154744-85-1P 154744-86-2P
154744-87-3P 154744-88-4P 154744-89-5P
154744-91-9P 154744-93-1P 154744-95-3P
154744-96-4P 154744-97-5P 154745-09-2P
154745-10-5P 154745-11-6P 154745-12-7P
154745-13-8P 154745-14-9P 154745-16-1P
154745-18-3P 154745-20-7P 154745-21-8P
154745-22-9P

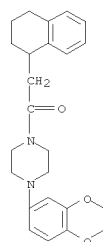
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as 5-HT receptor antagonist)

RN 154744-84-0 CAPLUS

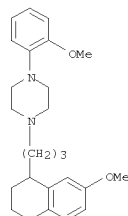
L25 ANSWER 70 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
1-naphthalenyl)- (CA INDEX NAME)



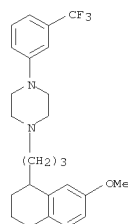
RN 161525-33-3 CAPLUS
CN Ethanone, 1-[4-(2,3-dihydro-1,4-benzodioxin-6-yl)-1-piperazinyl]-2-(
1,2,3,4-tetrahydro-1-naphthalenyl)- (CA INDEX NAME)



L25 ANSWER 71 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-
naphthalenyl)propyl]- (CA INDEX NAME)



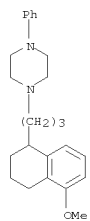
RN 154744-85-1 CAPLUS
CN Piperazine,
1-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]-4-[3-(
(trifluoromethyl)phenyl)- (CA INDEX NAME)



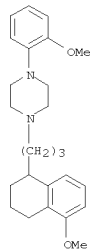
RN 154744-86-2 CAPLUS
CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-
naphthalenyl)propyl]- (CA INDEX NAME)

10590585.trn

L25 ANSWER 71 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

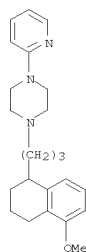


RN 154744-87-3 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)

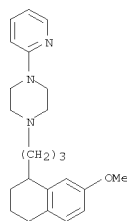


RN 154744-88-4 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)

L25 ANSWER 71 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

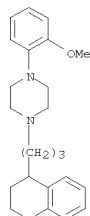


RN 154744-89-5 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]- (CA INDEX NAME)

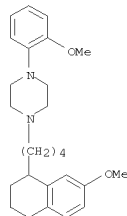


RN 154744-91-9 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-1-naphthalenyl)propyl]- (CA INDEX NAME)

L25 ANSWER 71 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

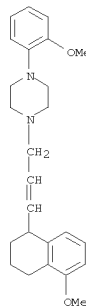


RN 154744-93-1 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[4-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)butyl]- (CA INDEX NAME)

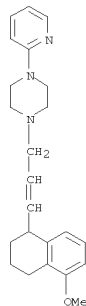


RN 154744-95-3 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)-2-propen-1-yl]- (CA INDEX NAME)

L25 ANSWER 71 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



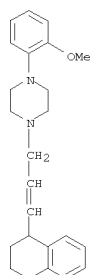
RN 154744-96-4 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)-2-propen-1-yl]- (CA INDEX NAME)



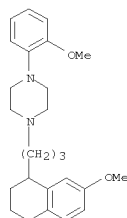
RN 154744-97-5 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-1-naphthalenyl)-2-propen-1-yl]- (CA INDEX NAME)

10590585.trn

L25 ANSWER 71 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



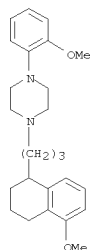
RN 154745-09-2 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]-, hydrochloride (1:?) (CA INDEX NAME)



●x HCl

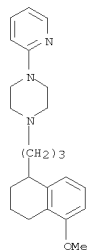
RN 154745-10-5 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:?) (CA INDEX NAME)

L25 ANSWER 71 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



●x HCl

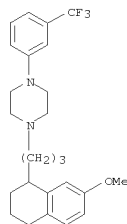
RN 154745-13-8 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]-, hydrochloride (1:?) (CA INDEX NAME)



●x HCl

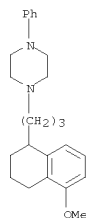
RN 154745-14-9 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[3-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)propyl]-, hydrochloride (1:?) (CA INDEX NAME)

L25 ANSWER 71 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



●x HCl

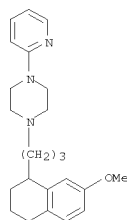
RN 154745-11-6 CAPLUS
CN Piperazine, 1-phenyl-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]-, hydrochloride (1:?) (CA INDEX NAME)



●x HCl

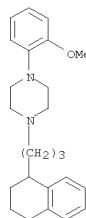
RN 154745-12-7 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)propyl]-, hydrochloride (1:?) (CA INDEX NAME)

L25 ANSWER 71 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



●x HCl

RN 154745-16-1 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-1-naphthalenyl)propyl]-, hydrochloride (1:?) (CA INDEX NAME)

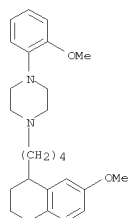


●x HCl

RN 154745-18-3 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[4-(1,2,3,4-tetrahydro-7-methoxy-1-naphthalenyl)butyl]-, hydrochloride (1:?) (CA INDEX NAME)

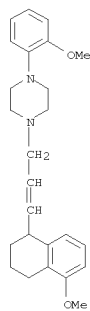
10590585.trn

L25 ANSWER 71 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



•x HCl

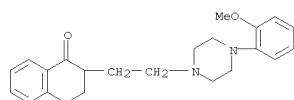
RN 154745-20-7 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)-2-propen-1-yl]-, hydrochloride (1:?) (CA INDEX NAME)



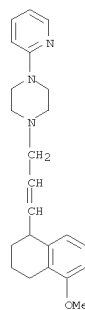
•x HCl

RN 154745-21-8 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-4-[3-(1,2,3,4-tetrahydro-5-methoxy-1-naphthalenyl)-2-propen-1-yl]-, hydrochloride (1:?) (CA INDEX NAME)

L25 ANSWER 72 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1993:485437 Document No. 119:85437 Original Reference No. 119:15093a,15096a
Antiserotonergic activity of 2-aminoethylbenzocyclanones in rat aorta: structure-activity relationships. Loza, M. I.; Ferreiro, T. G.; Sanz, F.; Lozoya, E.; Rodriguez, J.; Manaut, F.; Verde, I.; Castro, E.; Fontenla, J. A. (Dep. Pharmacol., Univ. Santiago, Santiago de Compostela, E-15706, Spain). Journal of Pharmaceutical Sciences, 82(5), 513-18 (English) 1993.
CODEN: JPMSAE. ISSN: 0022-3549.
AB The antiserotonergic activity at the serotonin receptor subtype 2 (5-HT₂) of seven new 2-aminoethylbenzocyclanones was determined with respect to serotonin-induced contractions in rat aorta and compared with that of ketanserin (pA₂ = 8.87). Competitive antagonism was observed in six compds. (6.72 ≤ pA₂ ≤ 8.12). Three-dimensional structures and mol. electrostatic potential distributions of ketanserin and 2-aminoethylbenzocyclanones were analyzed. Several mol. features correlated with the rank of antiserotonergic activity. In the case of the cyclanone fragment, the rank of activity was associated with the degree of planarity of the bicyclic system. The steric and electrostatic effects due to the loss of planarity were analyzed. In the case of the amino moiety, activity was associated with a particular spatial pattern defined by the amino nitrogen, the aromatic system, and mol. electrostatic potential min. generated by the oxygen atom.
IT 149247-12-1
RL: BIOL (Biological study)
(serotonergic S₂-antagonist activity of, in aorta, structure in relation to)
RN 149247-12-1 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[2-[4-(2-methoxyphenyl)-1-piperazinyl]ethyl]- (CA INDEX NAME)

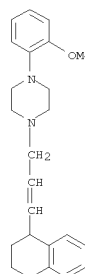


L25 ANSWER 71 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



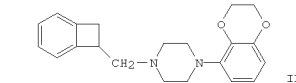
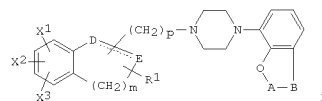
•x HCl

RN 154745-22-9 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(1,2,3,4-tetrahydro-1-naphthalenyl)-2-propen-1-yl]-, hydrochloride (1:?) (CA INDEX NAME)



•x HCl

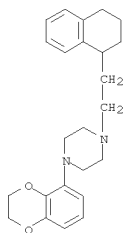
L25 ANSWER 73 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1992:551017 Document No. 117:1510170 Original Reference No. 117:26169a
1,4-Disubstituted piperazines, process for their preparation, and pharmaceutical compositions containing them as 5-HT_{1A} receptor antagonists. Peglioni, Jean Louis; Millan, Mark; Rivet, Jean Michel (Adir et Compagnie, Fr.). Eur. Pat. Appl. EP 490772 A1 19920617, 23 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE. (French). CODEN: EPXXDW. APPLICATION: EP 1991-403378 19911213. PRIORITY: FR 1990-15631 19901214.
GI



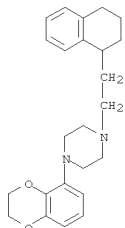
AB Title compds. I [X₁-X₃ = H, halo, alkyl, OH, alkoxy, alkylthio, CF₃, NO₂, amino, NHAc; or 2 of X form OCH₂O or OCH₂CH₂O; R₁ = H, alkyl; DE = (CH₂)_nCH₂ or CH₂CH₂; m, n = 0-3; m+n ≥ 1; p = 0-6; AB = (CH₂)₂O, (CH₂)₃O, CH₂CH₂, COCH₂CH₂], both racemic and optically active, are prepared for treatment of central nervous and neuroendocrine disorders (anxiety, depression, psychosis, diabetes, etc.). For example, N-alkylation of N-(benzodioxan-5-yl)piperazine by (benzocyclobutan-1-yl)methyl iodide and Na₂CO₃ in MIBK gave (after crystallization from iso-Pr₂O) 29% racemic title compound II. In an in vitro test for binding to rat hippocampal 5-HT_{1A} receptors (displacement of [3H]-8-OH-DPAT), pK_i was 8.74 for II and 7.93 for buspirone. Addnl. data include 28 synthetic examples, and in vivo animal experiment results (tail flick, body posture, corticosterone secretion, and hypothermia) for selected I.
IT 143355-89-9P 168329-98-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as 5-HT_{1A} antagonist)
RN 143355-89-9 CAPLUS
CN Piperazine, 1-(2,3-dihydro-1,4-benzodioxin-5-yl)-4-[2-(1,2,3,4-tetrahydro-1-naphthalenyl)ethyl]- (CA INDEX NAME)

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L25 ANSWER 73 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 168329-98-4 CAPLUS
CN Piperazine,
1-(2,3-dihydro-1,4-benzodioxin-5-yl)-4-[2-(1,2,3,4-tetrahydro-
1-naphthalenyl)ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

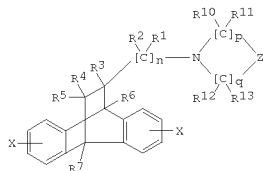


● HCl

IT 143356-23-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for 5-HT1A antagonist)
RN 143356-23-4 CAPLUS
CN Ethanone, 1-[4-(2,3-dihydro-1,4-benzodioxin-5-yl)-1-piperazinyl]-2-
(1,2,3,4-tetrahydro-1-naphthalenyl)- (CA INDEX NAME)

L25 ANSWER 74 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1992:51593 Document No. 116:515930 Original Reference No. 116:8751a,8754a
Use of bridged tricyclic amine derivatives for treating neurodegenerative
disorders and neurotoxic injury. Gray, Nancy M.; Contreras, Patricia C.
(G.D. Searle and Co., USA). U.S. US 5055468 A 19911008, 23 pp.
(English). CODEN: USXXAM. APPLICATION: US 1989-428531 19891030.

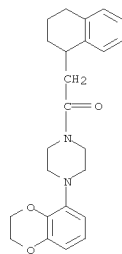
GI



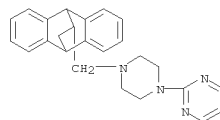
AB A neurodegenerative disorder or neurotoxic injury is treated by
administering a therapeutically effective amount of bridged tricyclic
amine
derivs. I (R1, R2 = H, alkyl, cycloalkyl, aryl, halo, etc.; R3-7 = H,
alkyl, OH, cycloalkyl, aralkyl, alkoxy, halo, etc.; n = 0-5; X = H, OH,
alkyl, halo, CN, etc.; R10-13 = H, alkyl, cycloalkyl, halo, etc.; R1 and
R2, R4 and R5, R10 and R11, R12 and R13 may form oxo; p,q = 1-4; Z = O,
S,
NR18; R18 = H, alkyl, cycloalkyl, etc., or R18 and 1 of R10-13 may form
fused 5-8-membered heterocycle ring) or a pharmaceutically-acceptable
salt. 4-[(9,10-Dihydro-9,10-ethanoanthracen-11-yl)methyl]-1-methylpiperazine
(II) (25 µg) blocked the effect of D-serine (200 µg) on cGMP in mice
cerebellum. Cell loss in gerbils was reduced by 30 mg II/kg in a
forebrain ischemia assay. II was prepared from anthracene and allyl
alc. in
3 steps.

IT 133960-68-6P 133960-71-1P 138142-15-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for treatment of neurodegenerative disorder and
neurotoxic
injury)
RN 133960-68-6 CAPLUS
CN Pyrimidine, 2-[4-[(9,10-dihydro-9,10-ethanoanthracen-11-yl)methyl]-1-
piperazinyl]-, hydrochloride (1:2) (CA INDEX NAME)

L25 ANSWER 73 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

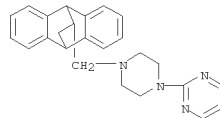


L25 ANSWER 74 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

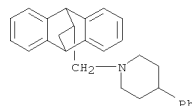


● 2 HCl

RN 133960-71-1 CAPLUS
CN Pyrimidine, 2-[4-[(9,10-dihydro-9,10-ethanoanthracen-11-yl)methyl]-1-
piperazinyl]- (CA INDEX NAME)



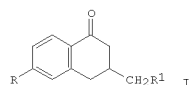
RN 138142-15-1 CAPLUS
CN Piperidine,
1-[[(9,10-dihydro-9,10-ethanoanthracen-11-yl)methyl]-4-phenyl-
(CA INDEX NAME)



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L25 ANSWER 75 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1991:449616 Document No. 115:496160 Original Reference No. 115:8617a,8620a
 Synthesis and antidopaminergic activity of some 3-(aminomethyl)tetralones
 as analogs of butyrophenone. Cortizo, Lourdes; Santana, Lourdes; Ravina,
 Enrique; Orallo, Francisco; Fontenla, Jose A.; Castro, Elena; Calleja,
 Jose M.; De Ceballos, Maria L. (Fac. Pharm., Univ. Santiago de
 Compostela,
 Santiago de Compostela, 15706, Spain). Journal of Medicinal Chemistry,
 34(7), 2242-7 (English) 1991. CODEN: JMCMAR. ISSN: 0022-2623. OTHER
 SOURCES: CASREACT 115:49616.

GI

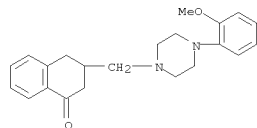


AB Starting from (β -benzoyl)propionic acid, e.g.,
 3-(aminomethyl)tetralones, e.g., I [R = F, R1 =
 4-(N-piperazinyl)-p-fluorobutyrophenone (II); R = H, R1 =
 4-benzoylpiperidin-1-yl (III)], 4-hydroxy-4-phenylpiperidin-1-yl,
 2-(methoxyphenyl)piperazinyl were synthesized. The possible dopamine
 antagonist activity of these compds. was investigated in both in vitro
 and in vivo expts. These compds. potently inhibited [3H]spiperone binding to
 D2 striatal receptors and moderately inhibited [3H]SCH-23390 binding to

D1 striatal receptors (Kis in the nanomolar and micromolar ranges, resp.).
 Apomorphine-induced stereotypies and amphetamine group toxicity were
 antagonized, to different extents by the compds. under study, with a
 potency similar to that of haloperidol. Interestingly, no catalepsy was
 observed after administration of the new compds. (2-8 mg/kg). The most
 active compds. in vivo, II and III, possessed two butyrophenone
 pharmacophores. However, the tetralone moiety appeared not critical for
 their antidopaminergic activity, since all target compds. were less
 active than haloperidol.

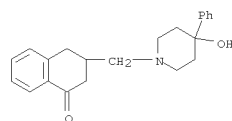
IT 133496-59-0P 133496-60-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and antidopaminergic activity of)
 RN 133496-59-0 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[(4-hydroxy-4-phenyl-1-
 piperidinyl)methyl]- (CA INDEX NAME)

L25 ANSWER 75 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

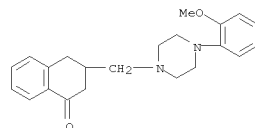


● 2 HCl

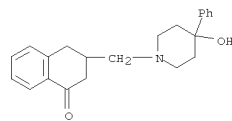
L25 ANSWER 75 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 133496-60-3 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[[4-(2-methoxyphenyl)-1-
 piperazinyl)methyl]- (CA INDEX NAME)



IT 133496-72-7P 133496-73-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 133496-72-7 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[(4-hydroxy-4-phenyl-1-
 piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

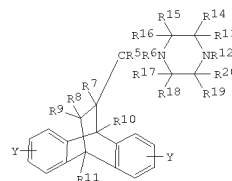


● HCl

RN 133496-73-8 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[[4-(2-methoxyphenyl)-1-
 piperazinyl)methyl]-, hydrochloride (1:2) (CA INDEX NAME)

L25 ANSWER 76 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1991:247300 Document No. 114:2473000 Original Reference No.
 114:41761a,41764a Preparation of dihetero nitrogen-containing
 cycloheteroethanoanthracene derivatives as antipsychotic agents. Gray,
 Nancy M. (G.D. Searle and Co., USA). Eur. Pat. Appl. EP 405436 A2
 19910102, 41 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB,
 GR, IT, LI, LU, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP
 1990-112113 19900626. PRIORITY: US 1989-374318 19890629.

GI



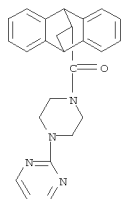
I

AB Title compds. I (R5, R6 = H, alkyl, PhCH2, Ph; R7 - R11 = H, alkyl, HO,
 PhCH2, Ph, alkoxy, PhO, PhCH2O, halo, haloalkyl; R12 = H, alkyl, C5-7
 cycloalkyl, Ph, PhCH2, hydroxyalkyl, C5-7 heterocyclyl; R13 - R20 = H,
 alkyl, PhCH2, Ph, halo, wherein R12 together with one of R13, R14, R19 or
 R20 may form a fused heterocyclyl containing 5-6-membered-ring) or a salt
 thereof, are prepared. I are also useful in treatment of convulsive and
 dystonic disorders. 11-(Bromomethyl)-9,10-dihydro-9,10-ethanoanthracene
 (preparation given), 1-methylpiperazine, and K2CO3 were combined in HMPA
 and heated to 90° for 48 h to give after workup I (R5 - R11, R13 - R20
 = Y = H, R12 = Me) (II). In blockade of agonist-induced stereotyped
 behavior and ataxia II blocked N-allylnormetazocine-induced stereotyped
 behavior and ataxia at 1 and 5 mg/kg, resp. In test for blockade of
 apomorphine-induced climbing, the ED50 of II was 1.0 mg/kg.

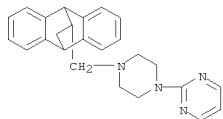
IT 133960-74-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reaction of, preparation of antipsychotics)
 RN 133960-74-4 CAPLUS
 CN Methanone, (9,10-dihydro-9,10-ethanoanthracen-11-yl)[4-(2-pyrimidinyl)-1-
 piperazinyl]- (CA INDEX NAME)

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L25 ANSWER 76 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



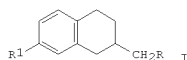
IT 133960-68-6P 133960-71-1P
 RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of, as antipsychotic)
 RN 133960-68-6 CAPLUS
 CN Pyrimidine, 2-[4-[(9,10-dihydro-9,10-ethanoanthracen-11-yl)methyl]-1-piperazinyl]-, hydrochloride (1:2) (CA INDEX NAME)



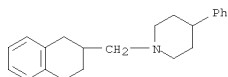
● 2 HCl

RN 133960-71-1 CAPLUS
 CN Pyrimidine, 2-[4-[(9,10-dihydro-9,10-ethanoanthracen-11-yl)methyl]-1-piperazinyl]- (CA INDEX NAME)

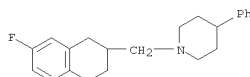
L25 ANSWER 77 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1990:191384 Document No. 112:191384 Original Reference No. 112:32149a
 Synthesis of 2-aminomethyltetralins as α -blocking and
 antidopaminergic agents. Santana, L.; Ravina, E.; Cortizo, L.; Orallo,
 F.
 (Dep. Quim. Org., Lab. Quim. Farm., Santiago de Compostela, 15706,
 Spain).
 Anales de la Real Academia de Farmacia, 55(4), 461-9 (Spanish) 1989.
 CODEN: ARAFAY. ISSN: 0034-0618.
 GI



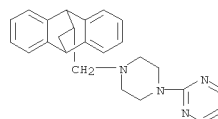
AB Five 2-aminomethyltetralins (I, R = heterocyclic; R1 = H, F) were
 prepared
 by reduction of corresponding 3-aminomethyl-1-tetralones. I were
 characterized by spectroscopic methods and tested for pharmacol. activity
 as α 1-adrenoblocking and antidopaminergic agents in preps. of the
 rat ductus deferens. Agents with the 4-phenylpiperidinyl substituents
 inhibited smooth muscle contractions induced by dopamine or noradrenaline
 to the extent similar to the action of haloperidol; the α 1-blocking
 activity was slightly weaker. The other agents had much weaker
 antidopaminergic effects and potentiated the contraction effects of
 noradrenaline. Details of structure-activity relations are discussed.
 IT 109132-90-3P 126684-48-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and antidopaminergic and α 1-adrenoblocking effects of,
 structure in relation to)
 RN 109132-90-3 CAPLUS
 CN Piperidine, 4-phenyl-1-[(1,2,3,4-tetrahydro-2-naphthalenyl)methyl]- (CA
 INDEX NAME)



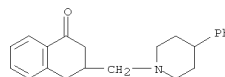
RN 126684-48-8 CAPLUS
 CN Piperidine, 1-[(7-Fluoro-1,2,3,4-tetrahydro-2-naphthalenyl)methyl]-4-phenyl- (CA INDEX NAME)



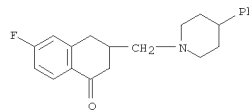
L25 ANSWER 76 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



L25 ANSWER 77 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 IT 126684-43-3 126684-44-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reduction of)
 RN 126684-43-3 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[(4-phenyl-1-piperidinyl)methyl]- (CA
 INDEX NAME)



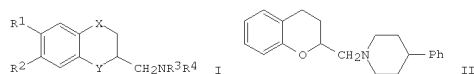
RN 126684-44-4 CAPLUS
 CN 1(2H)-Naphthalenone, 6-fluoro-3,4-dihydro-3-[(4-phenyl-1-piperidinyl)methyl]- (CA INDEX NAME)



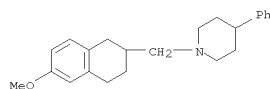
10590585.trn

L25 ANSWER 78 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1987:534201 Document No. 107:1342010 Original Reference No.
107:21677a,21680a Fungicidal benzopyran derivatives. Elliott, Alison
Clare; Anthony, Vivienne Margaret (Imperial Chemical Industries PLC, UK).
Ger. Offen. DE 3620408 A1 19861218, 49 pp. (German). CODEN: GWXXBX.
APPLICATION: DE 1986-3620408 19860618. PRIORITY: GB 1985-15389 19850618.

GI

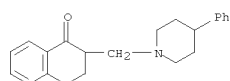


AB Benzopyrans I [X = CH₂, Y = O; X = O, Y = CH₂, CHOH; R₁, R₂ = H, halo, alkyl, alkenyl, alkynyl, alkoxy, haloalkyl, haloalkoxy; R₃, R₄ = C1-8 alkyl; NR₃R₄ = (un)substituted heterocyclyl] and their salts, useful as agrochem. fungicides, were prepared
3,4-Dihydro-1-benzopyran-2-carboxylic acid was converted with SOCl₂ to its acid chloride, which acylated 4-phenylpiperidine in CH₂Cl₂ containing pyridine and dimethylaminopyridine to give 100% N-(4-phenyl-1-piperidinyl)-3,4-dihydro-1-benzopyran-2-carboxamide. Reduction of this with LiAlH₄ in THF at 0° gave 80% benzopyran II. Barley inoculated with Erysiphe graminis was completely protected with 25 ppm II, and apple inoculated with Venturia inaequalis developed traces to 5% infection when treated with II. Wheat and peanuts developed 60-100% infection from Puccinia recondita and Cercospora arachidicola, resp., after inoculation and spraying with 25 ppm II.
IT RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as agrochem. fungicide)
RN 109132-64-1 CAPLUS
CN Piperidine, 4-phenyl-1-[(1,2,3,4-tetrahydro-6-methoxy-2-naphthalenyl)methyl]- (CA INDEX NAME)

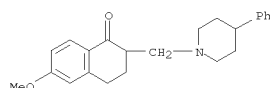


L25 ANSWER 79 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

RN 109132-87-8 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-phenyl-1-piperidinyl)methyl]- (CA INDEX NAME)

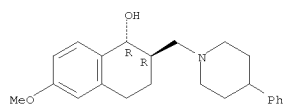


RN 109132-88-9 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[(4-phenyl-1-piperidinyl)methyl]- (CA INDEX NAME)

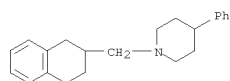


RN 109132-89-0 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-methoxy-2-[(4-phenyl-1-piperidinyl)methyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

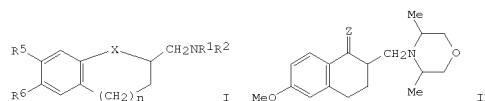


RN 109132-90-3 CAPLUS
CN Piperidine, 4-phenyl-1-[(1,2,3,4-tetrahydro-2-naphthalenyl)methyl]- (CA INDEX NAME)

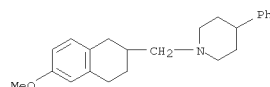


L25 ANSWER 79 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1987:439619 Document No. 107:396190 Original Reference No. 107:6619a,6622a
Fungicidal benzocycloalkylmethylamines. Worthington, Paul Anthony; Snell, Brian Kenneth; DeFraine, Paul; Anthony, Vivienne Margaret (Imperial Chemical Industries PLC, UK). Ger. Offen. DE 3620356 A1 19861218, 44 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1986-3620356 19860618. PRIORITY: GB 1985-15390 19850618; GB 1986-5418 19860305.

GI



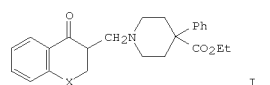
AB Fungicidal compns. comprised compds. I [R₅, R₆ = H, alkyl, alkoxy, when 1 of R₅ and R₆ = H, the other ≠ CMe₂R (R = H, Me, Et); X = CO or a derivative thereof, CR₃R₄, CR₃OR₄; R₃, R₄ = H, C1-4 alkyl; R₁, R₂ = H, C1-4 alkyl; NR₁R₂ = heterocyclyl; n = 0, 1] and a carrier. I were also prepared
6-Methoxy-1,2,3,4-tetrahydro-1-naphthalenone, 2,6-dimethylmorpholine-HCl, and paraformaldehyde were refluxed 3 h in EtOH containing catalytic HCl to give 33% tetrahydronaphthalenone II (Z = O), which was reduced with Zn-Hg to give 20% II (Z = H₂). No infection resulted when wheat was sprayed with 100 ppm II (Z = H₂) inoculated later with Puccinia recondita or when barley was inoculated with Puccinia recondita or when barley was inoculated with Erysiphe hordei graminis, then sprayed with II (Z = H₂). There was 60-100% infection with Cercospora arachidicola on peanuts and Pyricularia oryzae on rice and 26-59% infection with Venturia inaequalis on apples.
IT 109132-64-1P 109132-87-8P 109132-88-9P
109132-89-0P 109132-90-3P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn of, as agrochem. fungicide)
RN 109132-64-1 CAPLUS
CN Piperidine, 4-phenyl-1-[(1,2,3,4-tetrahydro-6-methoxy-2-naphthalenyl)methyl]- (CA INDEX NAME)



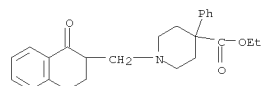
L25 ANSWER 80 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1987:196210 Document No. 106:196210 Original Reference No. 106:31801a,31804a

Synthesis of nor-meperidine derivatives with a possible analgetic and neuroleptic action. Kolokouris, N. M.; Lambrou, D. (Lab. Pharm. Chem., Univ. Athens, Athens, Greece). Chimika Chronika, 14(4), 251-5 (French) 1985. CODEN: CMCRZ. ISSN: 0366-693X.

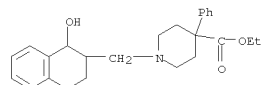
GI



AB The mannich bases I (X = CH₂, O, NMe) were prepared from normeperidine and were reduced to the alcs. The latter, according to P.A.J. Janssen (1970), have the required characteristics for neuroleptic and analgesic activity.
IT 108045-97-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and catalytic reduction of)
RN 108045-97-2 CAPLUS
CN 4-Piperidinecarboxylic acid, 4-phenyl-1-[(1,2,3,4-tetrahydro-1-oxo-2-naphthalenyl)methyl]-, ethyl ester (CA INDEX NAME)



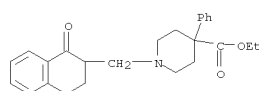
IT 108046-00-0P 108046-03-3P 108046-06-6P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
RN 108046-00-0 CAPLUS
CN 4-Piperidinecarboxylic acid, 4-phenyl-1-[(1,2,3,4-tetrahydro-1-hydroxy-2-naphthalenyl)methyl]-, ethyl ester (CA INDEX NAME)



RN 108046-03-3 CAPLUS
CN 4-Piperidinecarboxylic acid, 4-phenyl-1-[(1,2,3,4-tetrahydro-1-oxo-2-naphthalenyl)methyl]-, ethyl ester, hydrochloride (1:1) (CA INDEX NAME)

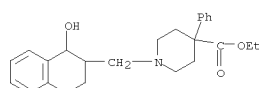
10590585.trn

L25 ANSWER 80 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● HCl

RN 108046-06-6 CAPLUS
CN 4-Piperidinecarboxylic acid, 4-phenyl-1-[(1,2,3,4-tetrahydro-1-hydroxy-2-naphthalenyl)methyl]-, ethyl ester, hydrochloride (1:1) (CA INDEX NAME)

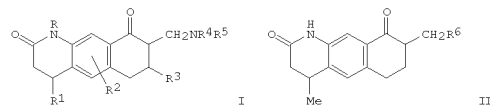


● HCl

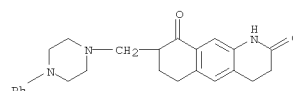
L25 ANSWER 81 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1986:148763 Document No. 104:148763 Original Reference No.
104:23545a,23548a

Benzo[g]quinoline derivatives. Nakao, Tatsu; Terasawa, Michio; Tawara, Tetsuya (Yoshitomi Pharmaceutical Industries, Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 60237071 A 19851125 Showa, 5 pp. (Japanese). CODEN: JKKXAF. APPLICATION: JP 1984-91615 19840507.

GI



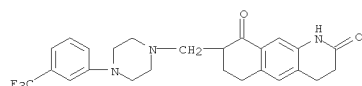
AB Title compds. I (R, R1, R3 = H, lower alkyl; R2 = H, lower alkyl, halo; R4, R5 = H, lower alkyl, aralkyl, alicyclic alkyl; or NR4R5 = heterocyclyl) and their salts, useful as cardiovascular agents, platelet aggregation inhibitors, analgesics, and antiinflammatory agents (no data), were prepared. Thus, 7.2 g II (R6 = H) was added to a mixture of N-methylpiperazine.2HCl 7.8 g, 3 mL 37% HCHO, and 30 mL acetic anhydride, then heated at 60-70° for 3 h to give 3.5 g II (R6 = N-methylpiperazino).2HCl.
IT 101237-44-9P 101237-45-0P 101237-46-1P
101237-47-2P 101237-48-3P 101237-49-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as cardiovascular agent, platelet aggregation inhibitor, analgesic, and antiinflammatory agent)
RN 101237-44-9 CAPLUS
CN Benzo[g]quinoline-2,9-dione, 1,3,4,6,7,8-hexahydro-8-[(4-phenyl-1-piperazinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

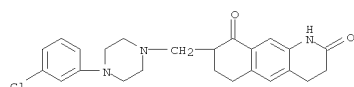
L25 ANSWER 81 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

RN 101237-45-0 CAPLUS
CN Benzo[g]quinoline-2,9-dione, 1,3,4,6,7,8-hexahydro-8-[[4-(3-(trifluoromethyl)phenyl)-1-piperazinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



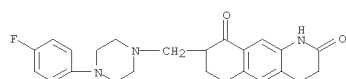
● HCl

RN 101237-46-1 CAPLUS
CN Benzo[g]quinoline-2,9-dione, 8-[[4-(3-chlorophenyl)-1-piperazinyl)methyl]-1,3,4,6,7,8-hexahydro-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

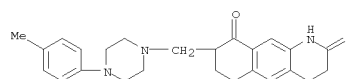
RN 101237-47-2 CAPLUS
CN Benzo[g]quinoline-2,9-dione, 8-[[4-(4-fluorophenyl)-1-piperazinyl)methyl]-1,3,4,6,7,8-hexahydro-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

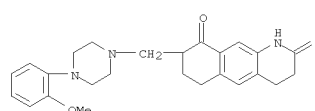
RN 101237-48-3 CAPLUS
CN Benzo[g]quinoline-2,9-dione, 1,3,4,6,7,8-hexahydro-8-[[4-(4-methylphenyl)-1-piperazinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 81 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● HCl

RN 101237-49-4 CAPLUS
CN Benzo[g]quinoline-2,9-dione, 1,3,4,6,7,8-hexahydro-8-[[4-(2-methoxyphenyl)-1-piperazinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

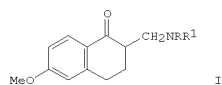


● HCl

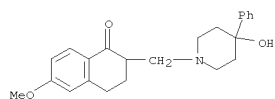
10590585.trn

L25 ANSWER 82 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1982;509663 Document No. 97:1096630 Original Reference No. 97:18233a,18236a
 Studies on the amine exchange reactions in C-Mannich bases. Kulkarni, Y.
 D.; Agarwal, Vipin Kumar (Dep. Chem., Univ. Lucknow, Lucknow, 226 007,
 India). Journal of the Indian Chemical Society, 59(3), 380-2 (English)
 1982. CODEN: JICSAH. ISSN: 0019-4522. OTHER SOURCES: CASREACT
 97:109663.

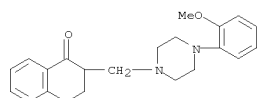
GI



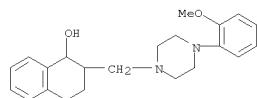
AB I (R = R1 = Me) and its methiodide underwent amine exchange reactions
 yielding I (RR1N = morpholino, 1-piperidinyl, p-ClC6H4NH, p-MeC6H4NH).
 IT 60682-02-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 60682-02-2 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-
 piperidinyl)methyl]-6-methoxy- (CA INDEX NAME)



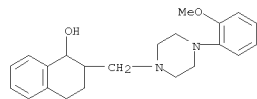
L25 ANSWER 83 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 IT 59646-26-3P 62811-21-6P 69644-05-9P
 69644-06-0P 69644-07-1P 69644-08-2P
 69644-09-3P 69644-10-6P 69644-11-7P
 69644-12-8P 69644-15-1P 69644-16-2P
 69644-17-3P 69644-19-5P 69644-20-8P
 69846-95-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 59646-26-3 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-(2-methoxyphenyl)-1-
 piperazinylmethyl]- (CA INDEX NAME)



RN 62811-21-6 CAPLUS
 CN 1-Naphthalenol, 1,2,3,4-tetrahydro-2-[[4-(2-methoxyphenyl)-1-
 piperazinylmethyl]- (CA INDEX NAME)



RN 69644-05-9 CAPLUS
 CN 1-Naphthalenol, 1,2,3,4-tetrahydro-2-[[4-(2-methoxyphenyl)-1-
 piperazinylmethyl]-, hydrochloride (1:1) (CA INDEX NAME)



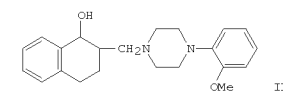
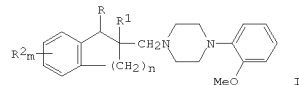
● HCl

RN 69644-06-0 CAPLUS
 CN 1-Naphthalenol, 1,2,3,4-tetrahydro-2-[[4-(2-methoxyphenyl)-1-
 piperazinylmethyl]-, cis- (9CI) (CA INDEX NAME)

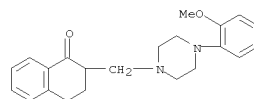
Relative stereochemistry.

L25 ANSWER 83 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1979;152239 Document No. 90:1522390 Original Reference No. 90:24209a,24212a
 1,2,3,4-Tetrahydro-2-((4-(phenyl)-1-piperazinyl)methyl)-1-naphthalenols
 and derivatives and analogs. Vogt, B. Richard; Cullison, David A. (E. R.
 Squibb and Sons, Inc., USA). U.S. US 4130646 19781219, 18 pp.
 (English).
 CODEN: USXXAM. APPLICATION: US 1976-679411 19760422.

GI

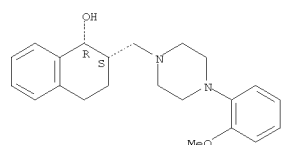


AB Piperazine derivs. I (R = OH, acyloxy; R1 = H; RR1 = bond; R2 = H,
 halogen, OH, acyloxy, alkoxy, alkylthio, alkyl, CF3; m, n = 1, 2) were
 prepared for use as neuroleptics, sedatives, muscle relaxants,
 antidepressants, and antianxiety agents (no data). Thus,
 1-(2-methoxyphenyl)piperazine was treated with α-tetralone and CH2O
 and reduced with NaBH4 to give II.
 IT 59646-31-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reduction of)
 RN 59646-31-0 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-(2-methoxyphenyl)-1-
 piperazinylmethyl]-, hydrochloride (1:2) (CA INDEX NAME)



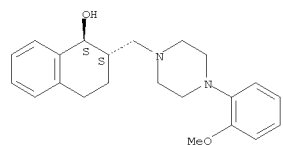
● 2 HCl

L25 ANSWER 83 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



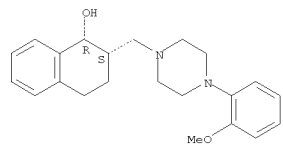
RN 69644-07-1 CAPLUS
 CN 1-Naphthalenol, 1,2,3,4-tetrahydro-2-[[4-(2-methoxyphenyl)-1-
 piperazinylmethyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 69644-08-2 CAPLUS
 CN 1-Naphthalenol, 1,2,3,4-tetrahydro-2-[[4-(2-methoxyphenyl)-1-
 piperazinylmethyl]-, dihydrochloride, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



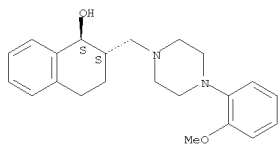
● 2 HCl

RN 69644-09-3 CAPLUS
 CN 1-Naphthalenol, 1,2,3,4-tetrahydro-2-[[4-(2-methoxyphenyl)-1-
 piperazinylmethyl]-, monohydrochloride, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

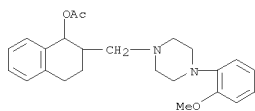
10590585.trn

L25 ANSWER 83 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



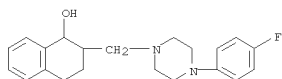
● HCl

RN 69644-10-6 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-, 1-acetate, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

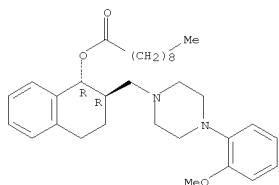
RN 69644-11-7 CAPLUS
CN 1-Naphthalenol, 2-[[4-(4-fluorophenyl)-1-piperazinyl]methyl]-1,2,3,4-tetrahydro-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 69644-12-8 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-6-methoxy-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-, hydrochloride (1:1) (CA INDEX NAME)

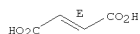
L25 ANSWER 83 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

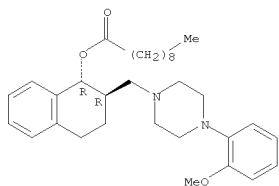


RN 69644-17-3 CAPLUS
CN Decanoic acid, (1R,2R)-1,2,3,4-tetrahydro-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-1-naphthalenyl ester, rel-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 69644-15-1
CMF C32 H46 N2 O3

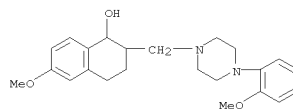
Relative stereochemistry.



CM 2

CRN 110-16-7

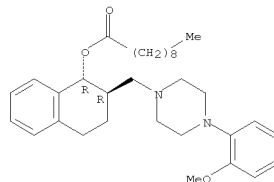
L25 ANSWER 83 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● HCl

RN 69644-15-1 CAPLUS
CN Decanoic acid, 1,2,3,4-tetrahydro-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-1-naphthalenyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 69644-16-2 CAPLUS
CN Decanoic acid, (1R,2R)-1,2,3,4-tetrahydro-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-1-naphthalenyl ester, rel-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

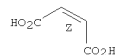
CM 1

CRN 69644-15-1
CMF C32 H46 N2 O3

Relative stereochemistry.

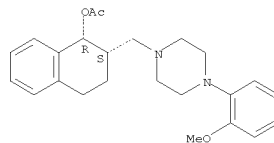
L25 ANSWER 83 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
CMF C4 H4 O4

Double bond geometry as shown.



RN 69644-19-5 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-, acetate (ester), dihydrochloride, cis- (9CI) (CA INDEX NAME)

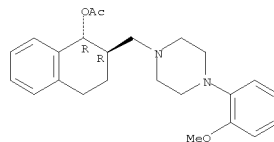
Relative stereochemistry.



● 2 HCl

RN 69644-20-8 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-, acetate (ester), dihydrochloride, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

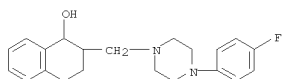


● 2 HCl

RN 69846-95-3 CAPLUS
CN 1-Naphthalenol, 2-[[4-(4-fluorophenyl)-1-piperazinyl]methyl]-1,2,3,4-tetrahydro- (CA INDEX NAME)

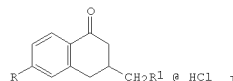
10590585.trn

L25 ANSWER 83 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

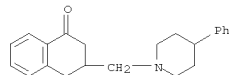


L25 ANSWER 84 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1979:151858 Document No. 90:1518580 Original Reference No. 90:24129a,24132a
Synthesis of 3-aminomethyl-1-tetralones as potential neuroleptic agents.
Eirin, Ana Maria; Santana, Lourdes; Ravina, Enrique; Fernandez, Franco;
Sanchez-Abarca, Eladio; Calleja, Jose Maria (Dep. Org. Pharm. Chem.,
Univ. Santiago de Compostela, Santiago, Spain). European Journal of Medicinal
Chemistry, 13(6), 533-7 (English) 1978. CODEN: EJMCA5. ISSN: 0009-4374.
OTHER SOURCES: CASREACT 90:151858.

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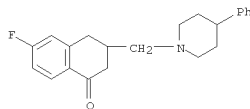
AB Tetralones I (R = H, R1 = 1-piperidinyl, 4-morpholinyl,
4-methyl-1-piperidinyl, 4-phenyl-1-piperidinyl; R = F, R1 =
4-phenyl-1-piperidinyl) were prepared by Mannich reaction of
m-RC6H4COCH2CH2CO2H with heterocyclic amines, catalytic reduction of the
resultant m-RC6H4COCH(CH2R1)CH2CO2H, followed by cyclization of the
products with polyphosphoric acid. Neuroleptic activity of I was
evaluated in mice by the following tests: variation of spontaneous motor
activity, hypothermia, evasion, rotating rod, traction, and chimney test;
in the 1st test all I had ED50 superior to 40 mg/kg.
IT 69797-43-9P 69797-44-0P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological
study); PREP (Preparation)
(preparation and neuroleptic activity of)
RN 69797-43-9 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-3-[(4-phenyl-1-piperidinyl)methyl]-,
hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 69797-44-0 CAPLUS
CN 1(2H)-Naphthalenone, 6-fluoro-3,4-dihydro-3-[(4-phenyl-1-
piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

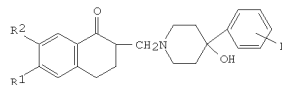
L25 ANSWER 84 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



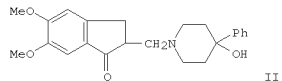
● HCl

L25 ANSWER 85 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1977:502172 Document No. 87:102172 Original Reference No. 87:16215a,16218a
Tetralone and indanone derivatives. (Merck Patent G.m.b.H., Fed. Rep.
Ger.). Neth. Appl. NL 7601762 19760824, 31 pp. (Dutch). CODEN: NAXXAN.
APPLICATION: NL 1976-1762 19760220.

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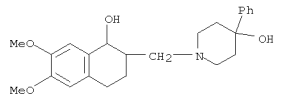


I



II

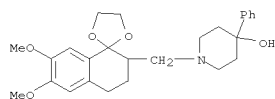
AB Piperidinomethyltetralones I (R = R2 = H, R1 = H, OH, O2Cet, CMe,
cyclopentyloxy; R = H, 4-Me, 4-F, 4-Cl, 3-CF3, 3,4-CF3Cl, R1 = R2 = OMe;
R = H, R1R2 = OCH2O) and indanone II were prepared by Mannich reaction. I
and II are central nervous system depressants, bactericides, and fungicides
(no data).
IT 60682-23-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of)
RN 60682-23-7 CAPLUS
CN 4-Piperidinol, 4-phenyl-1-[(1,2,3,4-tetrahydro-1-hydroxy-6,7-dimethoxy-2-
naphthalenyl)methyl]- (CA INDEX NAME)



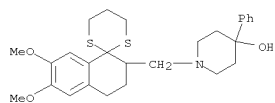
IT 60711-69-5P 60711-70-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and hydrolysis of)
RN 60711-69-5 CAPLUS
CN 4-Piperidinol, 1-[(3',4'-dihydro-6',7'-dimethoxyspiro[1,3-dioxolane-
2,1'(2'H)-naphthalen]-2'-yl)methyl]-4-phenyl- (CA INDEX NAME)

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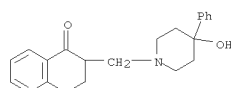
L25 ANSWER 85 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 60711-70-8 CAPLUS
CN 4-Piperidinol, 1-[(3',4'-dihydro-6',7'-dimethoxyspiro[1,3-dithiane-2,1'(2'H)-naphthalen]-2'-yl)methyl]-4-phenyl- (CA INDEX NAME)



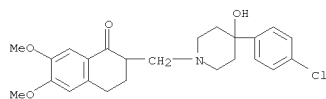
IT 60682-00-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)
RN 60682-00-0 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

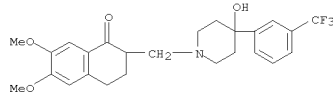
IT 60682-01-1P 60682-02-2P 60682-05-5P
60682-06-6P 60682-08-8P 63579-71-5P
63579-72-6P 63579-73-7P 63579-74-8P
63579-75-9P 63579-76-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 60682-01-1 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-hydroxy-2-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]- (CA INDEX NAME)

L25 ANSWER 85 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



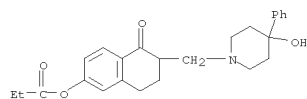
● HCl

RN 60682-08-8 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-hydroxy-4-[3-(trifluoromethyl)phenyl]-1-piperidinyl)methyl]-6,7-dimethoxy-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

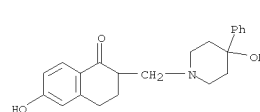
RN 63579-71-5 CAPLUS
CN 1-Naphthalenone, 1,2,3,4-tetrahydro-2-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-6-(1-oxopropoxy)-, hydrochloride (1:1) (CA INDEX NAME)



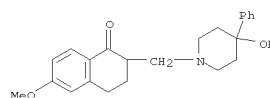
● HCl

RN 63579-72-6 CAPLUS
CN 1(2H)-Naphthalenone, 6-(cyclopentylloxy)-3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

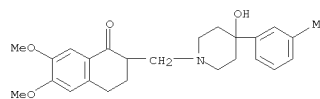
L25 ANSWER 85 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 60682-02-2 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-6-methoxy- (CA INDEX NAME)



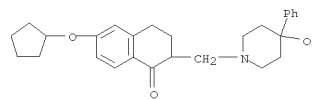
RN 60682-05-5 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-hydroxy-4-(3-methylphenyl)-1-piperidinyl)methyl]-6,7-dimethoxy-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

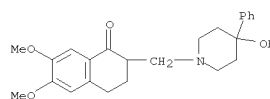
RN 60682-06-6 CAPLUS
CN 1(2H)-Naphthalenone, 2-[[4-(4-chlorophenyl)-4-hydroxy-1-piperidinyl)methyl]-3,4-dihydro-6,7-dimethoxy-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 85 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



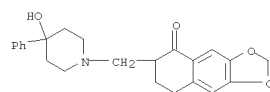
● HCl

RN 63579-73-7 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-6,7-dimethoxy-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 63579-74-8 CAPLUS
CN Naphtho[2,3-d]-1,3-dioxol-5(6H)-one, 7,8-dihydro-6-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

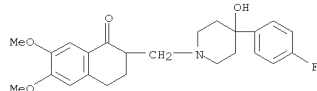


● HCl

RN 63579-75-9 CAPLUS
CN 1(2H)-Naphthalenone, 2-[[4-(4-fluorophenyl)-4-hydroxy-1-piperidinyl)methyl]-3,4-dihydro-6,7-dimethoxy-, hydrochloride (1:1) (CA INDEX NAME)

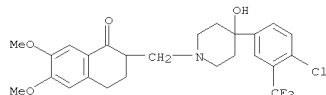
10590585.trn

L25 ANSWER 85 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● HCl

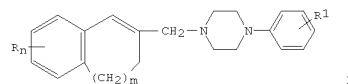
RN 63579-76-0 CAPLUS
CN 1(2H)-Naphthalenone,
2-[[4-[4-chloro-3-(trifluoromethyl)phenyl]-4-hydroxy-
1-piperidinyl]methyl]-3,4-dihydro-6,7-dimethoxy-, hydrochloride (1:1)
(CA INDEX NAME)



● HCl

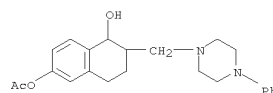
L25 ANSWER 86 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1977:406020 Document No. 87:6020 Original Reference No. 87:977a,980a
Phenylpiperazines. Vogt, Berthold R.; Cullison, David A. (E. R. Squibb
and Sons, Inc., USA). Ger. Offen. DE 2633214 19770217, 37 pp. (German).
CODEN: GWXXBX. APPLICATION: DE 1976-2633214 19760723.

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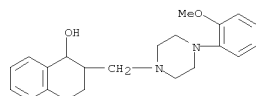
I

AB Phenylpiperazines [I; Rn, R1, m given: H, 2-MeO, 1; 5,6-(MeO)2, 2-MeO, 0;
H, 3-F3C, 1; 5,6-(MeO)2, 3-F3C, 0; H, 2-MeO, 0; H, 2-MeO, 2; 6-HO, H, 1],
useful as muscle relaxants and sedatives (no data), are prepared by known
methods. Thus, reaction of 170 g 1-(2-methoxyphenyl)piperazine-
hydrochloride with 172 g α-tetralone and 186 g 24% aqueous CH2O in
presence of concentrated HCl gives after .apprx.1 h 171 g
3,4-dihydro-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-1(2H)-
naphthalenone (II). Reduction of 2.14 g II.2HCl.1/2 H2O with NaBH4
gives 1.54
g 1,2,3,4-tetrahydro-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-1-
naphthalenol (III). Dehydration of 6 g III with AcOH-H2SO4 15 min at
100° gives 5.6 g I (Rn = H, R1 = 2-MeO, m = 1).
IT 62811-36-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of)
RN 62811-36-3 CAPLUS
CN 1,6-Naphthalenediol,
1,2,3,4-tetrahydro-2-[[4-phenyl-1-piperazinyl]methyl]-
6-acetate (CA INDEX NAME)

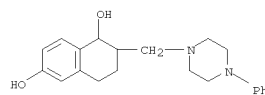


IT 62811-21-6P 62811-35-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and dehydration of)
RN 62811-21-6 CAPLUS
CN 1-Naphthalenol, 1,2,3,4-tetrahydro-2-[[4-(2-methoxyphenyl)-1-
piperazinyl]methyl]- (CA INDEX NAME)

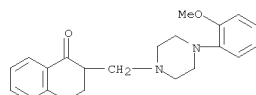
L25 ANSWER 86 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 62811-35-2 CAPLUS
CN 1,6-Naphthalenediol,
1,2,3,4-tetrahydro-2-[[4-phenyl-1-piperazinyl]methyl]-
(CA INDEX NAME)

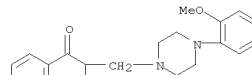


IT 59646-26-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reduction of)
RN 59646-26-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-(2-methoxyphenyl)-1-
piperazinyl]methyl]- (CA INDEX NAME)



IT 59646-31-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 59646-31-0 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-(2-methoxyphenyl)-1-
piperazinyl]methyl]-, hydrochloride (1:2) (CA INDEX NAME)

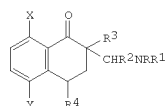
L25 ANSWER 86 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● 2 HCl

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L25 ANSWER 87 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1977:165067 Document No. 86:1650670 Original Reference No. 86:25852h,25853a
 Analgesic and tranquilizing activity of 5,8-disubstituted 1-tetralone
 Mannich bases. Welch, Willard M.; Harbert, Charles A.; Sarges, Reinhard;
 Stratten, Wilford P.; Weissman, Albert (Med. Res. Lab., Pfizer Inc.,
 Groton, CT, USA). Journal of Medicinal Chemistry, 20(5), 699-705
 (English) 1977. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES:
 CASREACT 86:165067.
 GI



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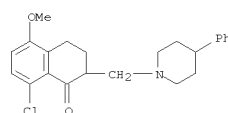
AB Forty-nine title compds. (including I: R, R1 = H, Me, Et, allyl, cyclohexyl; NRR1 = morpholino, piperidino, pyrrolidino, piperazino, azepino; R2 = H, Me, Ph; R3, R4 = H, Me; X = H, Cl, F, Me, OMe; Y = H, OMe, OEt) and 4 indanone analogs were prepared from the corresponding tetralones and indanones by standard Mannich reactions.
 8-Chloro-5-methoxy-2-morpholinomethyl-1-tetralone maleate [62491-08-1]

was the most potent neuroleptic agent with activity greater than thiothixene. Of the several compds. with analgesic activity, 8-chloro-5-methoxy-2-pyrrolidinomethyl-1-tetralone-HCl [62491-06-9] had potency in the morphine range and low neuroleptic activity, and gave no indication of tolerance development or cross tolerance to morphine, and was not reversed by naloxone. Structure-activity relations are discussed.

IT 62491-17-2P 62491-18-3P 62491-19-4P
 62491-20-7P 62491-21-8P 62491-22-9P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and analgesic activity of)

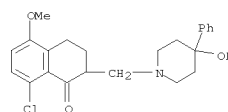
RN 62491-17-2 CAPLUS
 CN 1(2H)-Naphthalenone, 8-chloro-3,4-dihydro-5-methoxy-2-[(4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 87 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



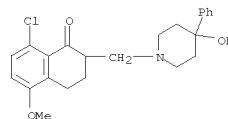
● HCl

RN 62491-18-3 CAPLUS
 CN 1(2H)-Naphthalenone, 8-chloro-3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-5-methoxy-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

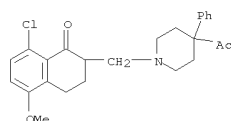
RN 62491-19-4 CAPLUS
 CN 1(2H)-Naphthalenone, 8-chloro-2-[(4-ethoxy-4-phenyl-1-piperidinyl)methyl]-3,4-dihydro-5-methoxy-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

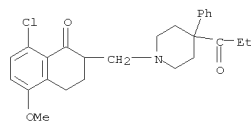
RN 62491-20-7 CAPLUS

L25 ANSWER 87 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
 CN 1(2H)-Naphthalenone, 2-[(4-acetyl-4-phenyl-1-piperidinyl)methyl]-8-chloro-3,4-dihydro-5-methoxy-, hydrochloride (1:1) (CA INDEX NAME)



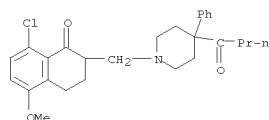
● HCl

RN 62491-21-8 CAPLUS
 CN 1(2H)-Naphthalenone, 8-chloro-3,4-dihydro-5-methoxy-2-[[4-(1-oxopropyl)-4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 62491-22-9 CAPLUS
 CN 1(2H)-Naphthalenone, 8-chloro-3,4-dihydro-5-methoxy-2-[[4-(1-oxobutyl)-4-phenyl-1-piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



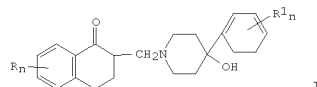
● HCl

L25 ANSWER 87 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

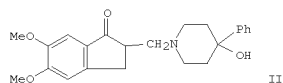
10590585.trn

L25 ANSWER 88 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1976:559908 Document No. 85:159908 Original Reference No. 85:25593a,25596a
 Tetralone and indanone derivatives of 4-piperidinol. Jonas, Rochus; Uhl,
 Juergen; Mueller-Calgan, Helmut; Irmacher, Klaus (Merck Patent G.m.b.H.,
 Fed. Rep. Ger.). Ger. Offen. DE 2507782 19760902, 42 pp. (German).
 CODEN: GWXXBX. APPLICATION: DE 1975-2507782 19750222.

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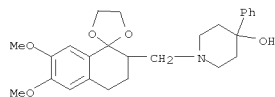


II

AB [(Hydroxypiperidino)methyl]tetralones [I; Rn = e.g., H, 6-OH, 6-MeO,
 6,7-(MeO)2, 6-NH2, 7-NO2; Rln = e.g., 3-Me, 4-Cl, 4-F, 3,4-(F3C)Cl],
 useful as central nervous depressants and antiemetics (no data), are
 prepared by several methods, predominantly by condensation of a tetralone
 with CH2O and a piperidinol. Thus, reaction of
 4-phenyl-4-piperidinol-hydrochloride with 1-tetralone and 37% CH2O in
 refluxing EtOH gives after 1 hr I.HCl (Rn = Rln = H). II is prepared
 similarly.

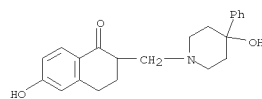
IT 60711-69-5 60711-70-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrolysis of)

RN 60711-69-5 CAPLUS
 CN 4-Piperidinol, 1-[(3',4'-dihydro-6',7'-dimethoxyspiro[1,3-dioxolane-
 2,1'(2'H)-naphthalen]-2'-yl)methyl]-4-phenyl- (CA INDEX NAME)

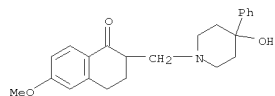


RN 60711-70-8 CAPLUS
 CN 4-Piperidinol, 1-[(3',4'-dihydro-6',7'-dimethoxyspiro[1,3-dithiane-
 2,1'(2'H)-naphthalen]-2'-yl)methyl]-4-phenyl- (CA INDEX NAME)

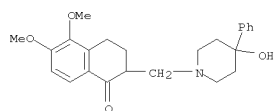
L25 ANSWER 88 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 60682-02-2 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-
 piperidinyl)methyl]-6-methoxy- (CA INDEX NAME)



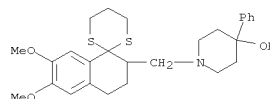
RN 60682-03-3 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-
 piperidinyl)methyl]-5,6-dimethoxy-, hydrochloride (1:1) (CA INDEX NAME)



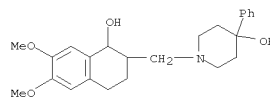
● HCl

RN 60682-04-4 CAPLUS
 CN Naphtho[1,2-d]-1,3-dioxol-6(7H)-one,
 8,9-dihydro-7-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-, hydrochloride
 (1:1) (CA INDEX NAME)

L25 ANSWER 88 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

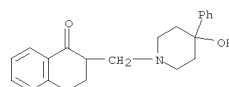


IT 60682-23-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of)
 RN 60682-23-7 CAPLUS
 CN 4-Piperidinol, 4-phenyl-1-[(1,2,3,4-tetrahydro-1-hydroxy-6,7-dimethoxy-2-
 naphthalenyl)methyl]- (CA INDEX NAME)



IT 60682-00-0P 60682-01-1P 60682-02-2P
 60682-03-3P 60682-04-4P 60682-05-5P
 60682-06-6P 60682-08-8P 60682-11-3P
 60682-12-4P 60682-13-5P 60682-14-6P
 60682-15-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

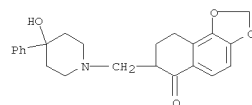
RN 60682-00-0 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-
 piperidinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

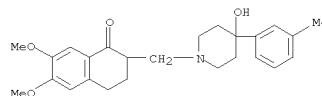
RN 60682-01-1 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-6-hydroxy-2-[(4-hydroxy-4-phenyl-1-
 piperidinyl)methyl]- (CA INDEX NAME)

L25 ANSWER 88 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



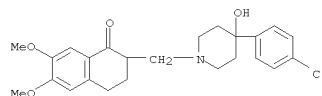
● HCl

RN 60682-05-5 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-hydroxy-4-(3-methylphenyl)-1-
 piperidinyl)methyl]-6,7-dimethoxy-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 60682-06-6 CAPLUS
 CN 1(2H)-Naphthalenone, 2-[[4-(4-chlorophenyl)-4-hydroxy-1-
 piperidinyl)methyl]-3,4-dihydro-6,7-dimethoxy-, hydrochloride (1:1) (CA
 INDEX NAME)

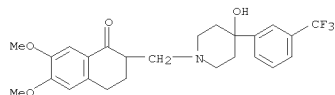


● HCl

RN 60682-08-8 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-hydroxy-4-[3-
 (trifluoromethyl)phenyl]-1-piperidinyl)methyl]-6,7-dimethoxy-,
 hydrochloride (1:1) (CA INDEX NAME)

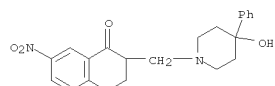
10590585.trn

L25 ANSWER 88 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

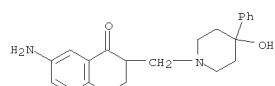


● HCl

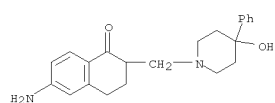
RN 60682-11-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]- (CA INDEX NAME)



RN 60682-12-4 CAPLUS
CN 1(2H)-Naphthalenone, 7-amino-3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]- (CA INDEX NAME)

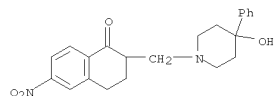


RN 60682-13-5 CAPLUS
CN 1(2H)-Naphthalenone, 6-amino-3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]- (CA INDEX NAME)



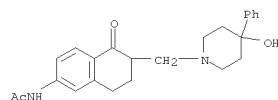
RN 60682-14-6 CAPLUS

L25 ANSWER 88 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

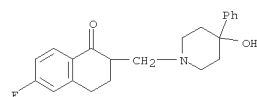


● HCl

L25 ANSWER 88 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
CN Acetamide, N-[5,6,7,8-tetrahydro-6-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-5-oxo-2-naphthalenyl]- (CA INDEX NAME)

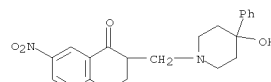


RN 60682-15-7 CAPLUS
CN 1(2H)-Naphthalenone, 6-fluoro-3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]- (CA INDEX NAME)



IT 60682-16-8 60682-17-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)

RN 60682-16-8 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-7-nitro-, hydrochloride (1:1) (CA INDEX NAME)

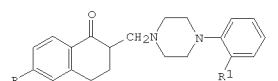


● HCl

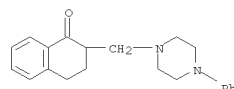
RN 60682-17-9 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-6-nitro-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 89 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1976:432952 Document No. 85:329520 Original Reference No. 85:5349a,5352a
Synthesis and potential neuroleptic activity of new Mannich bases derived from α -tetralone and N-arylpiperazines. Elrin, Ana M.; Ravina, Enrique; Montanes, Jose M.; Calleja, Jose M. (Fac. Pharm., Univ. Santiago Compostela, Santiago, Spain). European Journal of Medicinal Chemistry, 11(1), 29-32 (English) 1976. CODEN: EJMCAS. ISSN: 0223-5234. OTHER SOURCES: CASREACT 85:32952.

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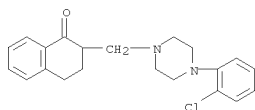
AB Five I (R = H, CMe; R1 = H, Cl, Me, OMe) were prepared by treating N-arylpiperazines with α -tetralones under Mannich reaction conditions. I (R = H, R1 = Cl) was reduced to the corresponding tetralol (II) with NaBH4. Neuroleptic activity of I and II was determined in mice; I with CMe or Cl groups had higher activity than others, and reduction of the keto group in I to alc. group in II decreased the activity.
IT 59646-23-0P 59646-24-1P 59646-25-2P
59646-26-3P 59646-27-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and neuroleptic activity)
RN 59646-23-0 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-phenyl-1-piperazinyl)methyl]- (CA INDEX NAME)



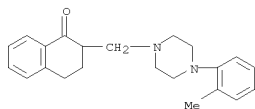
RN 59646-24-1 CAPLUS
CN 1(2H)-Naphthalenone, 2-[[4-(2-chlorophenyl)-1-piperazinyl)methyl]-3,4-dihydro- (CA INDEX NAME)

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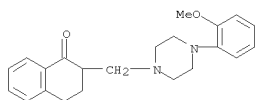
L25 ANSWER 89 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



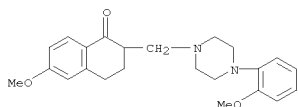
RN 59646-25-2 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-(2-methylphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



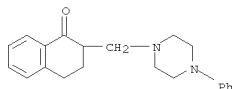
RN 59646-26-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



RN 59646-27-4 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)

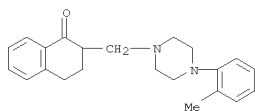


L25 ANSWER 89 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



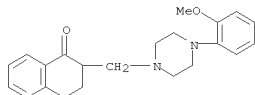
● 2 HCl

RN 59646-30-9 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-(2-methylphenyl)-1-piperazinyl]methyl]-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

RN 59646-31-0 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-, hydrochloride (1:2) (CA INDEX NAME)



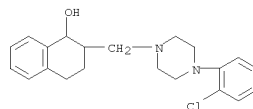
● 2 HCl

RN 59646-32-1 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-, hydrochloride (1:2) (CA INDEX NAME)

L25 ANSWER 89 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

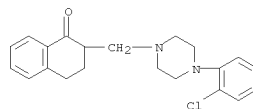
IT 59646-33-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation and neuroleptic activity of)

RN 59646-33-2 CAPLUS
CN 1-Naphthalenol, 2-[[4-(2-chlorophenyl)-1-piperazinyl]methyl]-1,2,3,4-tetrahydro- (CA INDEX NAME)



IT 59646-29-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reduction of)

RN 59646-29-6 CAPLUS
CN 1(2H)-Naphthalenone, 2-[[4-(2-chlorophenyl)-1-piperazinyl]methyl]-3,4-dihydro-, hydrochloride (1:2) (CA INDEX NAME)

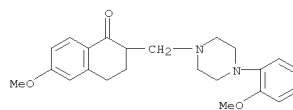


● 2 HCl

IT 59646-28-5P 59646-30-9P 59646-31-0P
59646-32-1P 59646-34-3P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

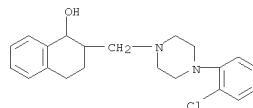
RN 59646-28-5 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-(phenyl-1-piperazinyl)methyl]-, hydrochloride (1:2) (CA INDEX NAME)

L25 ANSWER 89 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● 2 HCl

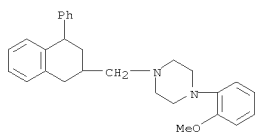
RN 59646-34-3 CAPLUS
CN 1-Naphthalenol, 2-[[4-(2-chlorophenyl)-1-piperazinyl]methyl]-1,2,3,4-tetrahydro-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

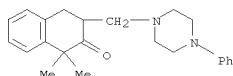
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L25 ANSWER 90 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1972:461675 Document No. 77:61675 Original Reference No. 77:10199a,10202a
 1-Phenyl-3-(aminoalkyl)-1,2,3,4-tetrahydronaphthalenes and their salts as
 anorectic agents or central nervous system stimulants. Holava, Henry
 Michael; Partyka, Richard Anthony (Bristol-Myers Co.). U.S. US 3663608
 19720516, 8 pp. (English). CODEN: USXXAM. APPLICATION: US 1969-883985
 19691210.
 GI For diagram(s), see printed CA Issue.
 AB -Phenyl-3-aminomethyl-1,2,3,4-tetrahydronaphthalenes (I) were prepared
 and
 found to have activity as anorectic agents or central nervous system
 stimulants. Thus, PhMgCl reacted with 3-carboxy-1-tetralone to give,
 after dehydration, 1-phenyl-3-carboxy-3,4-dihydronaphthalene, which was
 hydrogenated to II (R = H). II reacted with SOCl₂ and NH₃ or amines to
 give the corresponding amides which were treated with LiAlH₄ to give I.
 Among 17 I prepared as their hydrochloride salts were (R, R₁ given): H,
 H;
 H, Me; H, (CH₂)₃NMe₂; H, CH₂C.tplbond.CH; CF₃, Me. Also prepared were
 III
 and IV.
 IT 38046-29-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 38046-29-6 CAPLUS
 CN Piperazine, 1-(2-methoxyphenyl)-4-[(1,2,3,4-tetrahydro-4-phenyl-2-
 naphthalenyl)methyl]-, hydrochloride (1:2) (CA INDEX NAME)



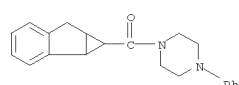
● 2 HCl

L25 ANSWER 92 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1967:37729 Document No. 66:37729 Original Reference No. 66:7175a,7178a
 Derivatives of 1- and 2-tetralones. DeStevens, George; Smolinsky,
 Barbara
 (CIBA Pharm Co., Summit, NJ, USA). Journal of Medicinal Chemistry, 9,
 954-7 (English) 1966. CODEN: JMCMAR. ISSN: 0022-2623.
 GI For diagram(s), see printed CA Issue.
 AB cf. CA 59, 2761h. Since 1-tetralone and 4-chromanone are useful in the
 synthesis of highly potent analgetics, some substituted derivs. are
 prepared
 especially with groups known to be responsible for particular boil.
 effects.
 The derivs. are obtained by condensation of the appropriate Grignard or
 organolithium reagent with the cycloketone. In this way I are prepared
 None of the compds. has any significant biol. activity. Since
 2-tetralone
 has a tendency to exist predominantly in the tautomeric form favoring
 enolization toward C-1, although some enolization toward C-3 also exists,
 1,1-dimethyl-2-tetralone derivs. were prepared to restrict reactivity to
 only one reactive center of the ketone. Also prepared are IV and VII.
 IT 7314-20-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 7314-20-7 CAPLUS
 CN 2(1H)-Naphthalenone, 3,4-dihydro-1,1-dimethyl-3-[(4-phenyl-1-
 piperazinyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)

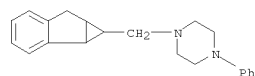


● HCl

L25 ANSWER 91 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1971:100100 Document No. 74:100100 Original Reference No. 74:16301a,16304a
 Antiinflammatory 1-[(N-heterocyclyl)methyl]-1a,2,3,7b-tetrahydro-1H-
 cyclopropa[a]naphthalenes and 1-[(N-heterocyclyl)methyl]-1,1a,6,6a-
 tetrahydrocycloprop[a]indenes. Welstead, William J., Jr. (A. H. Robins
 Co., Inc.). Ger. Offen. DE 2035400 19710204, 38 pp. (German). CODEN:
 GWXXBX. APPLICATION: DE 1970-2035400 19700716.
 GI For diagram(s), see printed CA Issue.
 AB The antiinflammatory title compds. (I, R = N-heterocyclyl; n = 1 or 2)
 were prepared Thus, reduction of trans-II with LiAlH₄ gave 67% trans-I
 [R =
 4-(p-chlorophenyl)-1,2,3,6-tetrahydro-1-pyridyl, n = 2; isolated as
 hydrochloride]. Similarly prepared were I (R, n, isomer, and salt
 isolated
 given): 3-phenyl-1-piperazinyl, 2, trans, -; 4-phenyl-1-piperazinyl, 1,
 trans, hydrochloride hydrate; 4-phenyl-1-piperazinyl, 2, cis, ;
 4-benzylpiperidino, 2, trans, hydrochloride,;
 4-(p-methoxyphenyl)-1-piperazinyl, 2, trans, hydrochloride;
 4-phenyl-1,2,3,6-tetrahydro-1-pyridyl, 2, trans, hydrochloride
 hemihydrate.
 IT 31481-70-6P 31481-75-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 31481-70-6 CAPLUS
 CN Piperazine, 1-phenyl-4-[(1,1a,6,6a-tetrahydrocycloprop[a]inden-1-
 yl)carbonyl]-, stereoisomer (8CI) (CA INDEX NAME)



RN 31481-75-1 CAPLUS
 CN Piperazine, 1-phenyl-4-[(1,1a,6,6a-tetrahydrocycloprop[a]inden-1-
 yl)methyl]-, monohydrochloride, stereoisomer (8CI) (CA INDEX NAME)

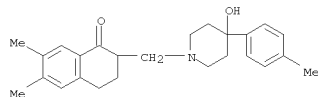


● HCl

L25 ANSWER 93 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1965:410079 Document No. 63:10079 Original Reference No. 63:1772d-h Benzyl
 piperidyl ketones. Pesson, Marcel (Laboratoire Roger Bellon). GB 979555
 19650106, 6 pp. (Unavailable). APPLICATION: GB 19620117. PRIORITY: GB
 19620117.
 GI For diagram(s), see printed CA Issue.
 AB The title compds., which have central nervous system activity, and in
 addition are either respiratory analectics or analgesics, were prepared
 by the
 condensation, in the presence of a basic catalyst, of a benzyl cyanide of
 the structure RC₆H₄CH₂CN with an ester of piperidinecarboxylic acid.
 Thus, a solution of 16 g. p-ethoxybenzyl cyanide and 25.4 g. ethyl
 N-methylisonipecotate in 40 cc. absolute alc. was added to a solution of
 EtONa
 (prepared from 3 g. Na and 60 cc. absolute EtOH) and refluxed 7 hrs. to
 yield
 8.5 g. α-(4-ethoxyphenyl)-α-N-methylisonipecotoylacetoneitrile
 (I), m. 239° (EtOH); HCl salt m. 142-4° (decomposition). A solution
 of 11.7 g. PhCH₂CN in 50 cc. PhMe was added to a suspension of NaNH₂
 [prepared from 2.3 g. Na and 200 cc. liquid NH₃ in the presence of a
 small
 quantity of Fe(NO₃)₃]. The excess NH₃ was driven off and 20.3 g. Et
 N-ethylisonipecotate was added and the mixture heated at 80° for 3
 hrs. to yield 21.1 g. α-phenyl-α-N-
 ethylisonipecotoylacetoneitrile, m. 274°; HCl salt m. 194°.
 The following acetonitriles were acetonitriles prepared (substituents and
 m.p.
 given): α-phenyl-α-N-methylpipecoloyl, -;
 α-phenyl-α-N-methylnipecotoyl (II), 255° [HCl salt m.
 161° (decomposition)]; α-(4-chlorophenyl)-N-methylnipecotoyl,
 256°; α-(4-chlorophenyl)-α-N-methylisonipecotoyl,
 306-7°; α-(4-chlorophenyl)-α-N-ethylisonipecotoyl,
 292°; α-phenyl-α-N-butylnipecotoyl, 197°;
 α-phenyl-α-N-methylisonipecotoyl, 297-80°. A solution of
 6 g. II in 60 cc. 2N NaOH was methylated in the usual manner with 9 cc.
 Me₂SO₄ to yield α-phenyl-α-methyl-α-N-
 methylnipecotoylacetoneitrile, m. 277°; HCl salt m. 238°. A
 suspension of 24.2 g. II in 50 cc. AcOH, 50 cc. H₂SO₄, and 25 cc. H₂O
 was refluxed 12 hrs., the bulk of the AcOH removed in vacuo on the H₂O bath,
 and the residue poured on to ice to yield 16.1 g. benzyl
 N-methyl-3-piperidyl ketone, b_{0.9} 135-40°; citrate m. 253°
 (EtOH). Hydrolysis of the corresponding oxonitriles similarly yielded
 the
 following ketones (m.p. given). 4-ClC₆H₄CH₂ N-methyl-3-piperidyl,
 71°; 4-ClC₆H₄CH₂ N-ethyl-4-piperidyl, 79°; PhCH₂
 N-ethyl-4-piperidyl, b_{0.8} 136-7° (HCl salt m. 174°);
 α-phenethyl N-methyl-3-piperidyl, - (citrate m. 228°); PhCH₂
 N-butyl-3-piperidyl, b_{0.8} 152-5° (oxalate m. 177°); PhCH₂
 N-methyl-4-piperidyl, b_{0.8} 140-2° [HCl salt m. 178° (EtOH)].
 IT 3036-57-5P, 1(2H)-Naphthalenone,
 3,4-dihydro-2-[(4-hydroxy-4-p-tolylpiperidino)methyl]-6,7-dimethyl-,
 hydrochloride
 RL: PREP (Preparation)
 (preparation of)
 RN 3036-57-5 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-hydroxy-4-(4-methylphenyl)-1-
 piperidinyl)methyl]-6,7-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)

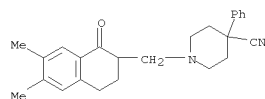
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L25 ANSWER 93 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



● HCl

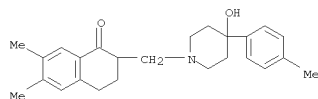
L25 ANSWER 94 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1965:410078 Document No. 63:10078 Original Reference No. 63:1772b-d
 β -Amino ketone derivatives. Nakanishi, Michio; Mukai, Toshihiko; Inamasu, Shuji (Yoshitomi Pharmaceutical Industries, Ltd.). JP 40006464 19650330 Showa, 2 pp. (Unavailable). APPLICATION: JP 19621130. PRIORITY: JP 19621130.
 GI For diagram(s), see printed CA Issue.
 AB Manufacture of I, a useful tranquilizer, was described. Thus, a mixture of 4-cyano-4-phenylpiperidine-HCl 2.23, paraformaldehyde 0.3, and 6,7-dimethyl-1-tetralone 1.75 g. is refluxed in 50 ml. EtOH containing small amount of HCl 7 hrs., then refluxed with more 0.15 g. paraformaldehyde 6 hrs., evaporated, the residue washed with dilute HCl, then washed with Et₂O, and recrystd. from dioxane-iso-PrOH to give I (R = CN, R' = Ph), m. 187-8°. Similarly is prepared I (R = OH, R' = p-tolyl), m. 167-7.5°.
 IT 3036-56-4P, Isonipecetonitrile, 1-phenyl-4-[(1,2,3,4-tetrahydro-6,7-dimethyl-1-oxo-2-naphthyl)methyl]-, hydrochloride 3036-57-5P, 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-hydroxy-4-p-tolylpiperidino)methyl]-6,7-dimethyl-, hydrochloride
 RL: PREP (Preparation)
 (preparation of)
 RN 3036-56-4 CAPLUS
 CN 4-Piperidinecarbonitrile, 4-phenyl-1-[(1,2,3,4-tetrahydro-6,7-dimethyl-1-oxo-2-naphthalenyl)methyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

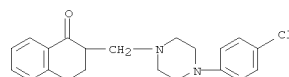
RN 3036-57-5 CAPLUS
 CN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-hydroxy-4-(4-methylphenyl)-1-piperidinyl)methyl]-6,7-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)

L25 ANSWER 94 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

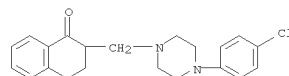


● HCl

L25 ANSWER 95 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
 1963:53341 Document No. 58:53341 Original Reference No. 58:9097g-h
Sulfamoyl-3,4-dihydro-4-quinazolones. Horii, Zenichi JP 37003580 19620606 Showa, 1 p. (Unavailable). APPLICATION: JP 19591125. PRIORITY: JP 19591125.
 GI For diagram(s), see printed CA Issue.
 AB A mixture of 0.3 g. 4-chloro-5-sulfamoylanthranilic acid and 1 cc. Formamide is heated at 160-5° for 1 hr., cooled, and allowed to stand with 5 cc. H₂O to give 0.25 g. (77%) 7-chloro-6-sulfamoyl-3,4-dihydro-4-quinazolinone (I), microneedles, m. 317-18° (decomposition) (H₂O). Also prepared is 7-sulfamoyl-3,4-dihydro-4-quinazolinone (m. 293-4°). These are useful as decarboxylase inhibitors.
 IT 94879-31-9P, 1(2H)-Naphthalenone, 2-[[4-(p-chlorophenyl)-1-piperazinyl)methyl]-3,4-dihydro-99904-89-9P, 1(2H)-Naphthalenone, 2-[[4-(p-chlorophenyl)-1-piperazinyl)methyl]-3,4-dihydro-, hydrobromide
 RL: PREP (Preparation)
 (preparation of)
 RN 94879-31-9 CAPLUS
 CN 1(2H)-Naphthalenone, 2-[[4-(4-chlorophenyl)-1-piperazinyl)methyl]-3,4-dihydro-, hydrobromide (1:7) (CA INDEX NAME)



RN 99904-89-9 CAPLUS
 CN 1(2H)-Naphthalenone, 2-[[4-(4-chlorophenyl)-1-piperazinyl)methyl]-3,4-dihydro-, hydrobromide (1:7) (CA INDEX NAME)

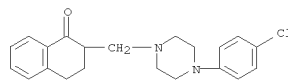


●x HBr

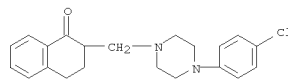
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L25 ANSWER 96 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN
1963;53340 Document No. 58;53340 Original Reference No. 58;9097c-g
N,N'-Disubstituted piperazines. Nichols, Gust (Miles Laboratories,
Inc.).
BE 614151 19620315, 17 pp. (Unavailable). PRIORITY: US 19610224.
GI For diagram(s), see printed CA Issue.
AB A series of HCl and HBr salts of disubstituted piperazines of the general
type I, where Y represents an α -oxocycloalkylmethyl group and R
stands for H, a halogen atom, or a lower alkyl or alkoxy group, is
described. N-Phenylpiperazine (II) (648 g.) in absolute EtOH treated
with 1 equivalent N alc. HBr (total volume of EtOH 3400 cc.), refluxed, treated
with 8 cc. concentrated HBr and 490 g. cyclohexanone (III) and then with 198 g.
paraformaldehyde in 25-g. portions during 45 min., refluxed 6.5 hrs.,
filtered hot, and cooled gave 903 g. 4-(2-oxocyclohexylmethyl)
derivative (IV)
of II.HBr, m. 168-70° (iso-PrOH). II (81 g.) in absolute EtOH
converted to II.HCl with alc. HCl (total volume of EtOH 500 cc.), treated
with 0.5 cc. concentrated HCl and 61.25 g. III and then dropwise with 55
cc. 37% aqueous CH₂O in 100 cc. absolute EtOH, and worked up the usual manner
yielded 76 g. IV.HCl, m. 167-8° (CHCl₃-C₆H₆). IV.HBr treated with K₂CO₃, and
the resulting IV treated with HCl gave IV.2HCl. In the usual manner were
prepared the following compds. (m.p. and starting amine and ketone
given):
4-(2-oxo-3-methylcyclohexylmethyl) derivative of II.HBr, 164-6° II,
2-methylcyclohexanone; 4-(2-oxo-5-methylcyclohexylmethyl) derivative of
II.HBr, 169-70°, II, 4-methylcyclohexanone;
4-(2-oxo-5-methoxycyclohexylmethyl) derivative of II.HBr, m. 154-5.5°
II, 4-methoxycyclohexanone; 1-(o-chlorophenyl)-4-(2-
oxocyclohexylmethyl)piperazine-HBr (V HBr), 171-3°,
N-(o-chlorophenyl)piperazine (VI), III; 1-(p-ClC₆H₄) analog of V.HBr,
173-4°, p-isomer of VI, III; 1-(p-MeC₆H₄) analog of V.HBr,
160-2°, N-(p-methylphenyl)piperazine, III.
N-(p-Chlo-phenyl)piperazine-HBr (VII.HBr) from 19.65 g. free base in 350
cc. absolute EtOH treated with 10.5 g. cyclopentanone and 0.25 cc.
concentrated HBr
and then during 80 min. with 5 g. paraformaldehyde, refluxed 3 hrs., and
worked up gave 12 g. 4-(2-oxocyclopentylmethyl) derivative of VII.HBr, m.
159-61° (EtOH). VII.HBr from 19.65 g. free base and 18.25 g.
1-tetralone gave 23 g. [1-(p-chlorophenyl)-4-piperazinylmethyl]-1-
tetralone-HBr, m. 192-4° (MeOH). Similarly was prepared
1-phenyl-4-(2-oxocyclopentylmethyl)piperazine-HBr, m. 158-60°. The
new piperazine derivs. show analgesic activity.
IT 94879-31-9P, 1(2H)-Naphthalenone,
2-[[4-(p-chlorophenyl)-1-piperazinyl]methyl]-3,4-dihydro-
99904-89-9P, 1(2H)-Naphthalenone,
2-[[4-(p-chlorophenyl)-1-piperazinyl]methyl]-3,4-dihydro-, hydrobromide
RL: PREP (Preparation)
(preparation of)
RN 94879-31-9 CAPLUS
CN 1(2H)-Naphthalenone, 2-[[4-(4-chlorophenyl)-1-piperazinyl]methyl]-3,4-
dihydro- (CA INDEX NAME)

L25 ANSWER 96 OF 96 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 99904-89-9 CAPLUS
CN 1(2H)-Naphthalenone, 2-[[4-(4-chlorophenyl)-1-piperazinyl]methyl]-3,4-
dihydro-, hydrobromide (1:7) (CA INDEX NAME)



●x HBr

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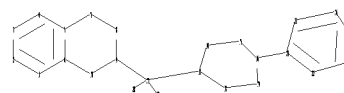
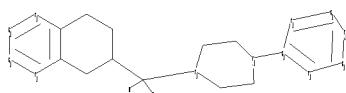
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chain nodes :

27

ring nodes :

1 2 3 4 5 6 7 8 9 10 13 14 15 16 18 19 20 21 22 23 25 26

ring/chain nodes :

28 29

chain bonds :

9-27 13-27 16-20 27-28 27-29

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 13-18 13-14 14-15 15-16
16-19 18-19 20-21 20-22 21-26 22-23 23-25 25-26

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 9-10 9-27 13-18 13-14 13-27 14-15
15-16 16-19 16-20 18-19 20-21 20-22 21-26 22-23 23-25 25-26 27-28 27-29

exact bonds :

7-8 8-9

10590585.trn

G1:C,N

Match level :

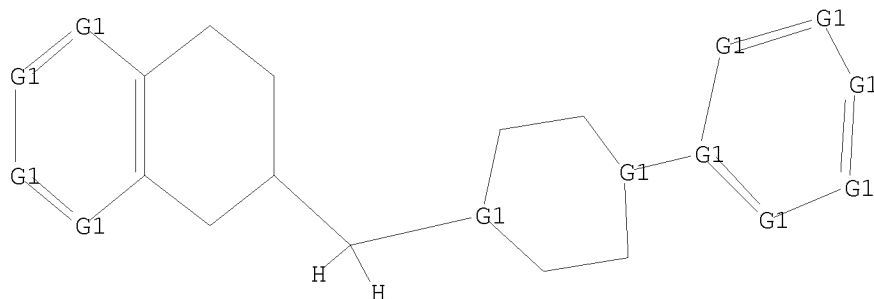
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
13:Atom 14:Atom 15:Atom 16:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS 29:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 C,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 16:52:25 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 79202 TO ITERATE

2.5% PROCESSED 2000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1567272 TO 1600808

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 16:52:30 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1587402 TO ITERATE

100.0% PROCESSED 1587402 ITERATIONS

265 ANSWERS

SEARCH TIME: 00.00.08

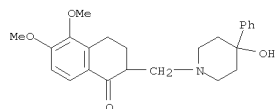
10590585.trn

L3 265 SEA SSS FUL L1

=> d scan

10590585.trn

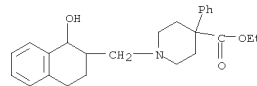
L3 265 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 1(2H)-Naphthalenone, 3,4-dihydro-2-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-5,6-dimethoxy-
MF C24 H29 N O4
CI CCM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

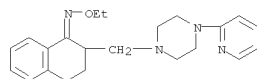
L3 265 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 4-Piperidinecarboxylic acid, 4-phenyl-1-[(1,2,3,4-tetrahydro-1-hydroxy-2-naphthalenyl)methyl]-, ethyl ester
MF C25 H31 N O3
CI CCM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

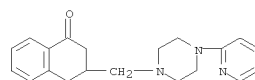
L3 265 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 1(2H)-Naphthalenone,
3,4-dihydro-2-[[4-(2-pyridinyl)-1-piperazinyl]methyl]-
, O-ethyloxime
MF C22 H28 N4 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 265 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 1(2H)-Naphthalenone,
3,4-dihydro-3-[[4-(2-pyridinyl)-1-piperazinyl]methyl]-
MF C20 H23 N3 O

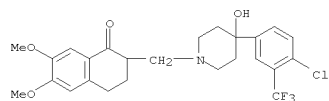


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

10590585.trn

L3 265 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 1(2H)-Naphthalenone,
 2-[[4-[4-chloro-3-(trifluoromethyl)phenyl]-4-hydroxy-
 1-piperidinyl]methyl]-3,4-dihydro-6,7-dimethoxy-, hydrochloride (1:1)
 MF C25 H27 Cl F3 N O4 . Cl H

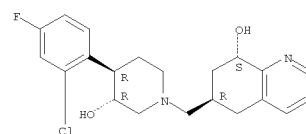


● HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 265 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 8-Quinololinol, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-
 piperidinyl]methyl]-5,6,7,8-tetrahydro-, hydrochloride (1:1), (6R,8S)-
 MF C21 H24 Cl F N2 O2 . Cl H

Absolute stereochemistry.

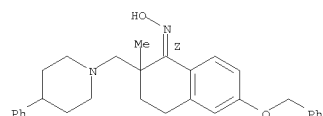


● HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 265 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 1(2H)-Naphthalenone,
 3,4-dihydro-2-methyl-6-(phenylmethoxy)-2-[(4-phenyl-1-
 piperidinyl)methyl]-, oxime, (1Z)-
 MF C30 H34 N2 O2

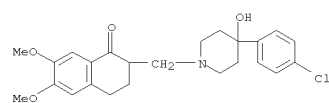
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 265 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 1(2H)-Naphthalenone, 2-[[4-(4-chlorophenyl)-4-hydroxy-1-
 piperidinyl]methyl]-3,4-dihydro-6,7-dimethoxy-, hydrochloride (1:1)
 MF C24 H28 Cl N O4 . Cl H

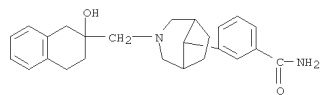


● HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

10590585.trn

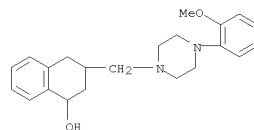
L3 265 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Benzanide, 3-[[3-[(1,2,3,4-tetrahydro-2-hydroxy-2-naphthalenyl)methyl]-3-azabicyclo[3.2.1]oct-8-yl]-
MF C25 H30 N2 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 265 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 1-Naphthalenol, 1,2,3,4-tetrahydro-3-[[4-(2-methoxyphenyl)-1-piperazinyl)methyl]-
MF C22 H28 N2 O2

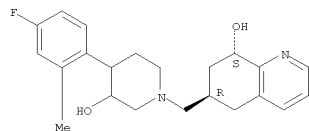


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

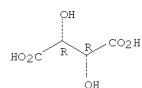
L3 265 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinololinol, 6-[[4-(4-fluoro-2-methylphenyl)-3-hydroxy-1-piperidinyl)methyl]-5,6,7,8-tetrahydro-, (6R,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1)
MF C22 H27 F N2 O2 . C4 H6 O6
CM 1

Absolute stereochemistry.



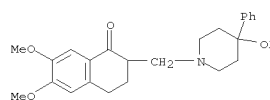
CM 2

Absolute stereochemistry.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 265 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 1(2H)-Naphthalenone, 3,4-dihydro-2-[[4-(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-6,7-dimethoxy-
MF C24 H29 N O4
CI CCM

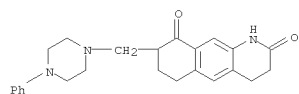


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

10590585.trn

L3 265 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Benzo[g]quinoline-2,9-dione, 1,3,4,6,7,8-hexahydro-8-[(4-phenyl-1-piperazinyl)methyl]-, hydrochloride (1:1)
MF C24 H27 N3 O2 . Cl H



● HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

10590585.trn

=> d his

(FILE 'HOME' ENTERED AT 16:51:53 ON 23 FEB 2010)

FILE 'REGISTRY' ENTERED AT 16:52:08 ON 23 FEB 2010

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 265 S L1 FULL

=> s l3 and C9N/rf

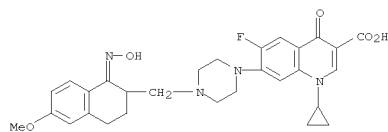
1566957 C9N/RF

L4 28 L3 AND C9N/RF

=> d scan

10590585.trn

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Quinolinescarboxylic acid,
 1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-[4-
 [(1,2,3,4-tetrahydro-1-(hydroxyimino)-6-methoxy-2-naphthalenyl)methyl]-1-
 piperazinyl]-
 MF C29 H31 F N4 O5

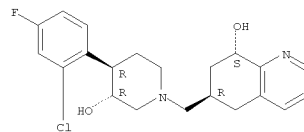


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2000

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 8-Quinololinol, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-
 piperidinyl)methyl]-5,6,7,8-tetrahydro-, (6R,8S)-
 MF C21 H24 Cl F N2 O2
 CI CCM

Absolute stereochemistry.

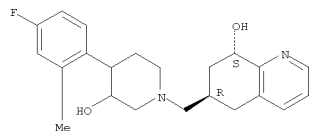


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 8-Quinololinol, 6-[[[4-(4-fluoro-2-methylphenyl)-3-hydroxy-1-
 piperidinyl)methyl]-5,6,7,8-tetrahydro-, (6R,8S)-,
 (2R,3R)-2,3-dihydroxybutanedioate (1:1)
 MF C22 H27 F N2 O2 . C4 H6 O6

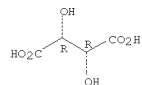
CM 1

Absolute stereochemistry.

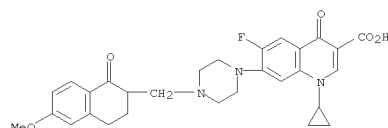


CM 2

Absolute stereochemistry.



L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Quinolinescarboxylic acid,
 1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-[4-
 [(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-piperazinyl]-
 MF C29 H30 F N3 O5



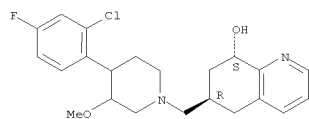
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10590585.trn

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinololinol, 6-[[4-(2-chloro-4-fluorophenyl)-3-methoxy-1-piperidinyl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (salt) (9CI)
MF C22 H26 Cl F N2 O2 . C4 H6 O6

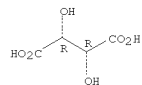
CM 1

Absolute stereochemistry.



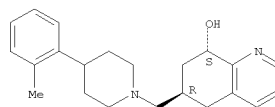
CM 2

Absolute stereochemistry.



L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinololinol, 5,6,7,8-tetrahydro-6-[[4-(2-methylphenyl)-1-piperidinyl]methyl]-, (6R,8S)-
MF C22 H28 N2 O
CI CCM

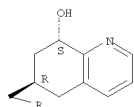
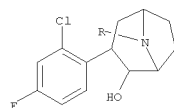
Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

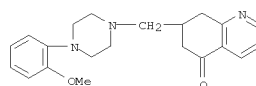
L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Azabicyclo[3.2.1]octan-2-ol, 3-(2-chloro-4-fluorophenyl)-8-[[(6R,8S)-5,6,7,8-tetrahydro-8-hydroxy-6-quinolinyl]methyl]-, hydrochloride (1:1)
MF C23 H26 Cl F N2 O2 . Cl H

Absolute stereochemistry.



● HCl

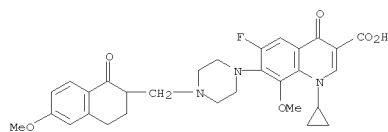
L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 5(6H)-Quinololinone, 7,8-dihydro-7-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-
MF C21 H25 N3 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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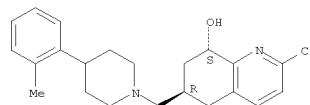
L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Quinolinescarboxylic acid,
1-cyclopropyl-6-fluoro-1,4-dihydro-8-methoxy-4-
oxo-7-[4-[(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-
piperazinyl]-
MF C30 H32 F N3 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinololinol, 2-chloro-5,6,7,8-tetrahydro-6-[[4-(2-methylphenyl)-1-
piperidinyl)methyl]-, (6R,8S)-rel-
MF C22 H27 Cl N2 O

Relative stereochemistry.

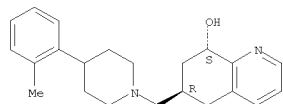


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinololinol, 5,6,7,8-tetrahydro-6-[[4-(2-methylphenyl)-1-
piperidinyl)methyl]-, (6R,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1)
MF C22 H28 N2 O . C4 H6 O6

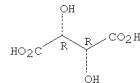
CM 1

Absolute stereochemistry. Rotation (-).



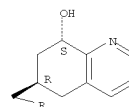
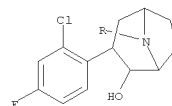
CM 2

Absolute stereochemistry.



L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Azabicyclo[3.2.1]octan-2-ol, 3-(2-chloro-4-fluorophenyl)-8-[[(6R,8S)-
5,6,7,8-tetrahydro-8-hydroxy-6-quinoliny]methyl]-
MF C23 H26 Cl F N2 O2
CI COM

Absolute stereochemistry.

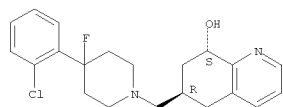


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10590585.trn

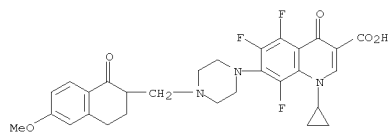
L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinololinol, 6-[[4-(2-chlorophenyl)-4-fluoro-1-piperidinyl]methyl]-
5,6,7,8-tetrahydro-, (6R,8S)-
MF C21 H24 Cl F N2 O
CI COM

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

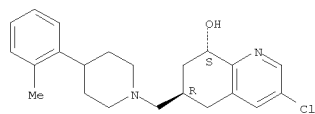
L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Quinolincarboxylic acid, 1-cyclopropyl-5,6,8-trifluoro-1,4-dihydro-4-
oxo-7-[[4-[(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-
piperazinyl]-
MF C29 H28 F3 N3 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinololinol, 3-chloro-5,6,7,8-tetrahydro-6-[[4-(2-methylphenyl)-1-
piperidinyl]methyl]-, (6R,8S)-rel-
MF C22 H27 Cl N2 O
CI COM

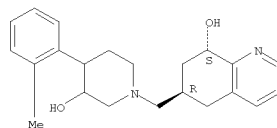
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinololinol, 5,6,7,8-tetrahydro-6-[[3-hydroxy-4-(2-methylphenyl)-1-
piperidinyl]methyl]-, (6R,8S)-
MF C22 H28 N2 O2
CI COM

Absolute stereochemistry.

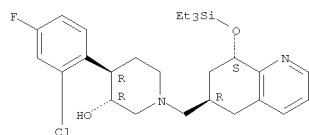


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10590585.trn

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Piperidinol,
4-(2-chloro-4-fluorophenyl)-1-[[[(6R,8S)-5,6,7,8-tetrahydro-
8-[(triethylsilyl)oxy]-6-quinolinyl)methyl]-, (3R,4R)-
MF C27 H38 Cl F N2 O2 S1

Absolute stereochemistry.

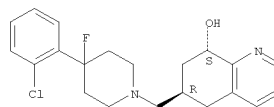


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinolinel, 6-[[[4-(2-chlorophenyl)-4-fluoro-1-piperidinyl)methyl]-
5,6,7,8-tetrahydro-, (6R,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1)
(salt) (9CI)
MF C21 H24 Cl F N2 O . C4 H6 O6

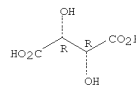
CM 1

Absolute stereochemistry.

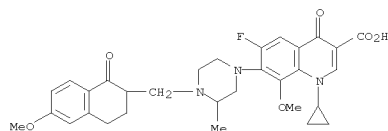


CM 2

Absolute stereochemistry.



L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Quinolinelcarboxylic acid,
1-cyclopropyl-6-fluoro-1,4-dihydro-8-methoxy-7-
[3-methyl-4-[(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-
piperazinyl]-4-oxo-
MF C31 H34 F N3 O6

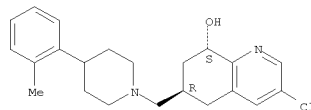


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinolinel, 3-chloro-5,6,7,8-tetrahydro-6-[[[4-(2-methylphenyl)-1-
piperidinyl)methyl]-, (6R,8S)-rel-, (2R,3R)-2,3-dihydroxybutanedioate
(1:1) (salt) (9CI)
MF C22 H27 Cl N2 O . C4 H6 O6

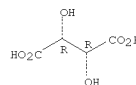
CM 1

Relative stereochemistry.



CM 2

Absolute stereochemistry.

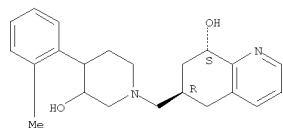


10590585.trn

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 8-Quinololinol, 5,6,7,8-tetrahydro-6-[[[3-hydroxy-4-(2-methylphenyl)-1-piperidinyl]methyl]-, (6R,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1)
 MF C22 H28 N2 O2 . C4 H6 O6

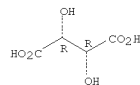
CM 1

Absolute stereochemistry.



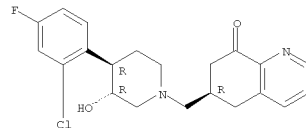
CM 2

Absolute stereochemistry.



L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 8(5H)-Quinololinone, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-piperidinyl]methyl]-6,7-dihydro-, (6R)-
 MF C21 H22 Cl F N2 O2

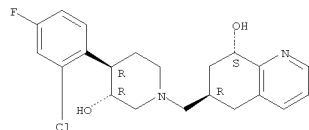
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

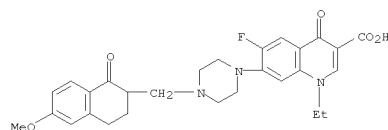
L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 8-Quinololinol, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-piperidinyl]methyl]-5,6,7,8-tetrahydro-, hydrochloride (1:1), (6R,8S)-
 MF C21 H24 Cl F N2 O2 . Cl H

Absolute stereochemistry.



● HCl

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
 IN 3-Quinolincarboxylic acid, 1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-[4-[(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-piperazinyl]-
 MF C28 H30 F N3 O5

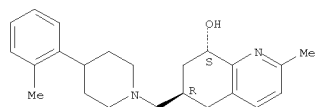


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10590585.trn

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinololinol, 5,6,7,8-tetrahydro-2-methyl-6-[[4-(2-methylphenyl)-1-piperidinyl]methyl]-, (6R,8S)-rel-
MF C23 H30 N2 O

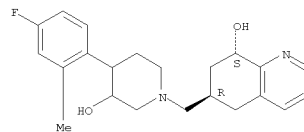
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinololinol, 6-[[4-(4-fluoro-2-methylphenyl)-3-hydroxy-1-piperidinyl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)-
MF C22 H27 F N2 O2
CI CCM

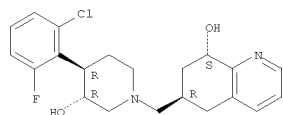
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinololinol, 6-[[[(3R,4R)-4-(2-chloro-6-fluorophenyl)-3-hydroxy-1-piperidinyl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)-
MF C21 H24 Cl F N2 O2

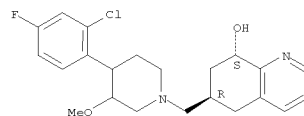
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinololinol, 6-[[4-(2-chloro-4-fluorophenyl)-3-methoxy-1-piperidinyl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)-
MF C22 H26 Cl F N2 O2
CI CCM

Absolute stereochemistry.



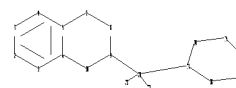
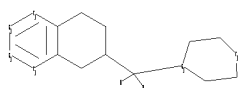
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

10590585.trn

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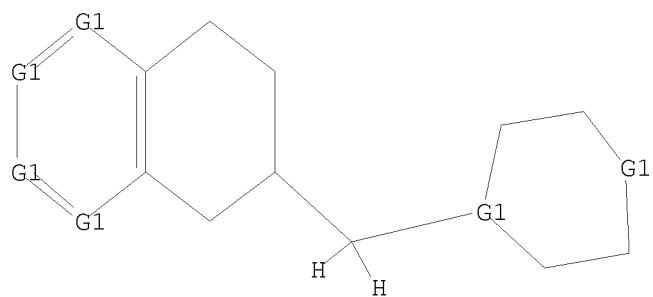
10590585.trn

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR



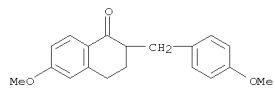
G1 C,N

Structure attributes must be viewed using STN Express query preparation.

=> s 15

10590585.trn

L6 3 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[(4-methoxyphenyl)methyl]-
MF C19 H20 O3



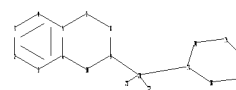
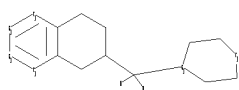
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

10590585.trn

=>

Uploading C:\Program Files\Stnexp\Queries\11580585-0000.str



chain nodes :

20

ring nodes :

1 2 3 4 5 6 7 8 9 10 13 14 15 16 18 19

ring/chain nodes :

21 22

chain bonds :

9-20 13-20 20-21 20-22

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 13-18 13-14 14-15 15-16
16-19 18-19

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 9-10 9-20 13-18 13-14 13-20 14-15
15-16 16-19 18-19 20-21 20-22

exact bonds :

7-8 8-9

G1:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
13:Atom 14:Atom 15:Atom 16:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS

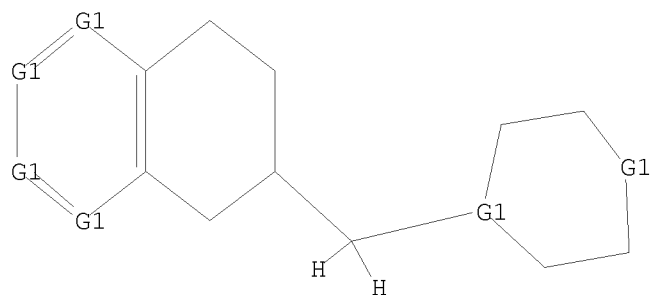
10590585.trn

L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR



G1 C,N

Structure attributes must be viewed using STN Express query preparation.

=> s 17

SAMPLE SEARCH INITIATED 16:55:46 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 79202 TO ITERATE

2.5% PROCESSED 2000 ITERATIONS

3 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1567272 TO 1600808

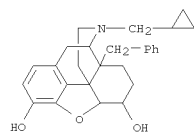
PROJECTED ANSWERS: 1723 TO 3029

L8 3 SEA SSS SAM L7

=> d scan

10590585.trn

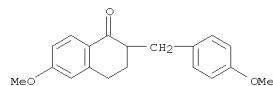
L8 3 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Morphinan-3,6-diol, 17-(cyclopropylmethyl)-4,5-epoxy-14-(phenylmethyl)-,
(5 α ,6 α)-(9CI)
MF C27 H31 N O3
CI CCM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

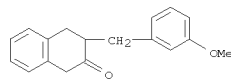
L8 3 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 1(2H)-Naphthalenone, 3,4-dihydro-6-methoxy-2-[(4-methoxyphenyl)methyl]-
MF C19 H20 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L8 3 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 2(1H)-Naphthalenone, 3,4-dihydro-3-[(3-methoxyphenyl)methyl]-
MF C18 H18 O2



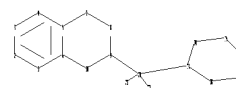
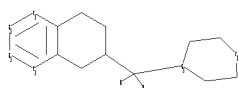
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

10590585.trn

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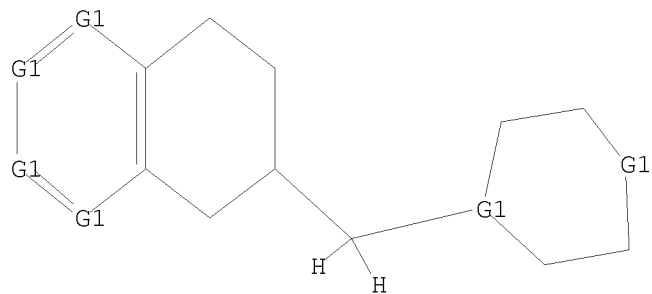
10590585.trn

L9 STRUCTURE UPLOADED

=> d 19

L9 HAS NO ANSWERS

L9 STR



G1 C,N

Structure attributes must be viewed using STN Express query preparation.

=> s 19

SAMPLE SEARCH INITIATED 16:57:07 FILE 'REGISTRY'

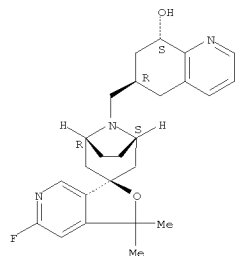
SAMPLE SCREEN SEARCH COMPLETED - 59389 TO ITERATE

10590585.trn

L12 45 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinololinol, 6-[[{(1R,5S)-6'-fluoro-1',1'-dimethylspiro[8-
azabicyclo[3.2.1]octane-3,3'-(1'H)-furo[3,4-c]pyridin]-8-yl)methyl]-5,6,7,8-
tetrahydro-, (6R,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (salt)
(9CI)
MF C25 H30 F N3 O2 . C4 H6 O6

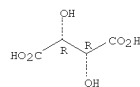
CM 1

Absolute stereochemistry.



CM 2

Absolute stereochemistry.

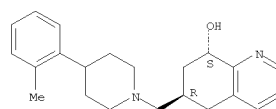


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L12 45 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinololinol, 5,6,7,8-tetrahydro-6-[[4-(2-methylphenyl)-1-
piperidinyl)methyl]-, (6R,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1)
MF C22 H28 N2 O . C4 H6 O6

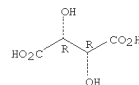
CM 1

Absolute stereochemistry. Rotation (-).



CM 2

Absolute stereochemistry.

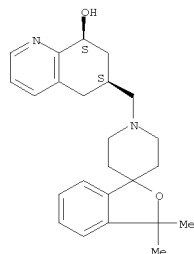


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L12 45 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinololinol, 6-[(3,3-dimethylspiro[isobenzofuran-1(3H),4'-piperidin]-1'-
yl)methyl]-5,6,7,8-tetrahydro-, (6S,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (salt) (9CI)
MF C24 H30 N2 O2 . C4 H6 O6

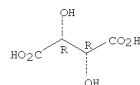
CM 1

Absolute stereochemistry.



CM 2

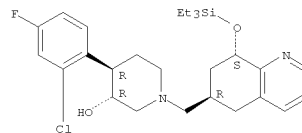
Absolute stereochemistry.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L12 45 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 3-Piperidinol, 4-(2-chloro-4-fluorophenyl)-1-[[{(6R,8S)-5,6,7,8-tetrahydro-
8-[(triethylsilyl)oxy]-6-quinolinyl)methyl]-, (3R,4R)-
MF C27 H38 Cl F N2 O2 Si

Absolute stereochemistry.



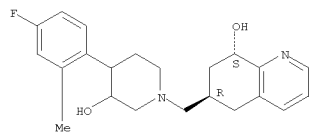
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

10590585.trn

L12 45 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinolinelol, 6-[[4-(4-fluoro-2-methylphenyl)-3-hydroxy-1-
piperidinyl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)-
MF C22 H27 F N2 O2
CI CCM

Absolute stereochemistry.

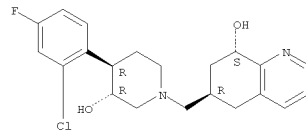


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L12 45 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8-Quinolinelol, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-
piperidinyl]methyl]-5,6,7,8-tetrahydro-, hydrochloride (1:1), (6R,8S)-
MF C21 H24 Cl F N2 O2 . Cl H

Absolute stereochemistry.

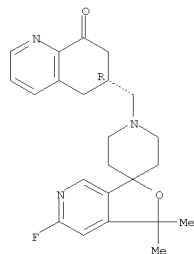


● HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L12 45 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 8(5H)-Quinololinone, 6-[(6-fluoro-1,1-dimethylspiro[furo[3,4-c]pyridine-
3(1H),4'-piperidin]-1'-yl)methyl]-6,7-dihydro-, (6R)-
MF C23 H26 F N3 O2

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

10590585.trn

=> file caplus

FILE 'CAPLUS' ENTERED AT 16:57:53 ON 23 FEB 2010

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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE LAST UPDATED: 22 Feb 2010 (20100222/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2009

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

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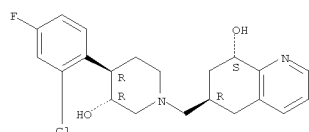
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YOU HAVE REQUESTED DATA FROM 9 ANSWERS - CONTINUE? Y/(N):y

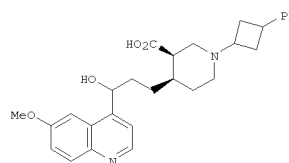
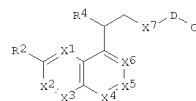
10590585.trn

L13 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN
2009:753543 Document No. 151:1632230 Identification of an Orally Active
Opioid Receptor-like 1 (ORL1) Receptor Antagonist

4-[3-[(2R)-2,3-Dihydroxypropyl]-2-oxo-2,3-dihydro-1H-benzimidazol-1-yl]-1-
[(1S,3S,4R)-spiro[bicyclo[2.2.1]heptane-2,1'-cyclopropan]-3-
ylmethyl]piperidine as Clinical Candidate. Satoh, Atsushi; Sagara,
Takeshi; Sakoh, Hiroki; Hashimoto, Masaya; Nakashima, Hiroshi; Kato,
Tetsuya; Goto, Yasuhiro; Mizutani, Sayaka; Azuma-Kanoh, Tomoko; Tani,
Takeshi; Okuda, Shoki; Okamoto, Osamu; Ozaki, Satoshi; Iwasawa,
Yoshikazu;
Ohta, Hisashi; Kawamoto, Hiroshi (Tsukuba Research Institute, Banyu
Pharmaceutical Co. Ltd., Okubo-3, Tsukuba 300-2611, Ibaraki, 300-2611,
Japan). Journal of Medicinal Chemistry, 52(14), 4091-4094 (English)
2009.
CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 151:163223.
Publisher: American Chemical Society.
AB Our efforts to optimize prototype opioid receptor-like 1 (ORL1)
antagonist
1 led to the discovery of 4-[3-[(2R)-2,3-dihydroxypropyl]-2-oxo-2,3-
dihydro-1H-benzimidazol-1-yl]-1-[(1S,3S,4R)-spiro[bicyclo[2.2.1]heptane-
2,1'-cyclopropan]-3-ylmethyl]piperidine 10. 10 Showed potent ORL1
antagonistic activity, excellent selectivity over other opioid receptors,
and in vivo efficacy after oral dosing. Currently clin. trials of 10 are
underway.
IT 864830-99-9
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(orally active ORL1 antagonists preparation)
RN 864830-99-9 CAPLUS
CN 8-Quinololinol, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-
piperidinyl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)- (CA INDEX NAME)
Absolute stereochemistry.

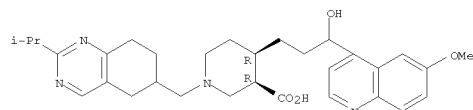


L13 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN
2008:1368162 Document No. 149:5566000 Substituted heterocyclic derivatives
as antimicrobial agents and their preparation, pharmaceutical
compositions
and use in the treatment of bacterial infection. Brickner, Steven
Jozseph;
Chen, Jinshan Michael; Li, Zhengong Bryan; Marfat, Anthony; Mitton-Fry,
Mark Joseph; Plotkin, Michael A.; Reilly, Usa Datta; Subramanyam,
Chakrapani; Zhang, Zhijun; Robinson, Shaughnessy (Pfizer Inc., USA).
U.S. Pat. Appl. Publ. US 20080280879 A1 20081113, 54pp. (English). CODEN:
USXXCO. APPLICATION: US 2008-117071 20080508. PRIORITY: US 2007-916906P
20070509.
GI

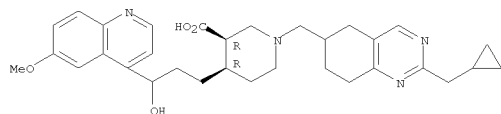


AB Comps. of the general formula I, their preparation and their use as
antimicrobial agents are disclosed. Comps. of formula I wherein at
least
one of X1 - X6 is N or N-oxide and the remaining is N and CR1; each R1 is
independently H, halo, CN, Cl-6 alkyl, Cl-6 alkoxy, etc.; R2 is H, OH,
halo, NH2, Cl-6 alkyl, Cl-6 alkylthio, etc.; X7 is O, NH and derivs.,
CH2,
S, SO, SO2, etc.; R4 is H, OH, Cl-6 alkoxy, F, NH2, CN, etc.; D is
(un)substituted azacycyl and (un)substituted azacycylalkyl; C is
(un)substituted cycloalkyl and (un)substituted azacycle; and
pharmaceutically acceptable salts, prodrugs, hydrates, and solvates
thereof, are claimed. Example compound II was prepared by a multistep
procedure (procedure given). All the invention comps. were evaluated
for

L13 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
their antimicrobial activity (data given).
IT 1080635-89-7P 1080635-90-0P 1080635-91-1P
1080635-92-2P 1080635-93-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation of substituted heterocyclic derivs. as antimicrobial
agents
useful in the treatment of bacterial infection)
RN 1080635-89-7 CAPLUS
CN 3-Piperidinecarboxylic acid, 4-[3-hydroxy-3-(6-methoxy-4-
quinolinyl)propyl]-1-[[[5,6,7,8-tetrahydro-2-(1-methylethyl)-6-
quinazolinyl]methyl]-, (3R,4R)- (CA INDEX NAME)
Absolute stereochemistry.

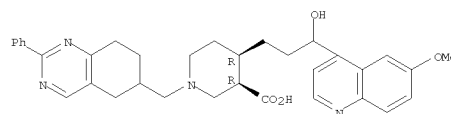


RN 1080635-90-0 CAPLUS
CN 3-Piperidinecarboxylic acid,
1-[[[2-(cyclopropylmethyl)-5,6,7,8-tetrahydro-
6-quinazolinyl]methyl]-4-[3-hydroxy-3-(6-methoxy-4-quinolinyl)propyl]-,
(3R,4R)- (CA INDEX NAME)
Absolute stereochemistry.

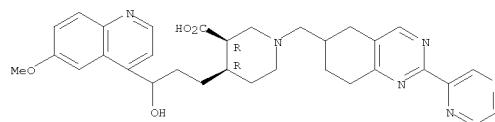


RN 1080635-91-1 CAPLUS
CN 3-Piperidinecarboxylic acid, 4-[3-hydroxy-3-(6-methoxy-4-
quinolinyl)propyl]-1-[[[5,6,7,8-tetrahydro-2-phenyl-6-quinazolinyl]methyl]-,
(3R,4R)- (CA INDEX NAME)
Absolute stereochemistry.

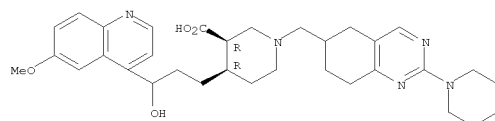
L13 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 1080635-92-2 CAPLUS
CN 3-Piperidinecarboxylic acid, 4-[3-hydroxy-3-(6-methoxy-4-
quinolinyl)propyl]-1-[[[5,6,7,8-tetrahydro-2-(2-pyrazinyl)-6-
quinazolinyl]methyl]-, (3R,4R)- (CA INDEX NAME)
Absolute stereochemistry.



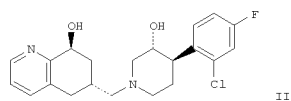
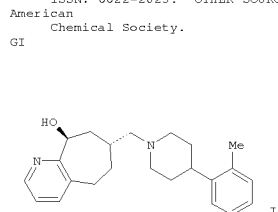
RN 1080635-93-3 CAPLUS
CN 3-Piperidinecarboxylic acid, 4-[3-hydroxy-3-(6-methoxy-4-
quinolinyl)propyl]-1-[[[5,6,7,8-tetrahydro-2-(1-piperidinyl)-6-
quinazolinyl]methyl]-, (3R,4R)- (CA INDEX NAME)
Absolute stereochemistry.



10590585.trn

L13 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN
2008:685859 Document No. 149:1761540 A Novel Class of
Cycloalkano[b]pyridines as Potent and Orally Active Opioid Receptor-like

1 Antagonists with Minimal Binding Affinity to the hERG K⁺ Channel.
Yoshizumi, Takashi; Takahashi, Hirobumi; Miyazoe, Hiroshi; Sugimoto,
Yuichi; Tsujita, Tomohiro; Kato, Tetsuya; Ito, Hirokatsu; Kawamoto,
Hiroshi; Hirayama, Miko; Ichikawa, Daisuke; Azuma-Kanoh, Tomoko; Ozaki,
Satoshi; Shibata, Yoshihiro; Tani, Takeshi; Chiba, Masato; Ishii,
Yasuyuki; Okuda, Shoki; Tadano, Kiyoshi; Fukuroda, Takahiro; Okamoto,
Osamu; Ohta, Hisashi (Tsukuba Research Institute, Banyu Pharmaceutical
Co., Ltd, Okubo-3, Tsukuba, Ibaraki, 300-2611, Japan). Journal of
Medicinal Chemistry, 51(13), 4021-4029 (English) 2008. CODEN: JMCMAR.
ISSN: 0022-2623. OTHER SOURCES: CASREACT 149:176154. Publisher:
American
Chemical Society.
GI



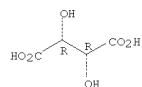
AB A series of compds. based on
7-([4-(2-methylphenyl)piperidin-1-yl]methyl)-
6,7,8,9-tetrahydro-5H-cyclohepta[b]pyridine-9-ol ((-)-I), a potent and
selective opioid receptor-like 1 (ORL1) antagonist, was prepared and
evaluated using structure-activity relationship studies with the aim of
removing its affinity to human ether-a-go-go related gene (hERG) K⁺
channel. From these studies, II was identified as an optimized structure
with respect to ORL1 antagonist activity, and affinity to the hERG
K⁺channel. Furthermore, II showed good in vivo antagonism with a wide
therapeutic index in regards to adverse cardiovascular effects.

IT 864828-68-2P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP
(Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL
(Biological study); PREP (Preparation); USES (Uses)
(crystal structure; synthesis and biol. evaluation of

L13 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CM 2
CRN 87-69-4
CMF C4 H6 O6

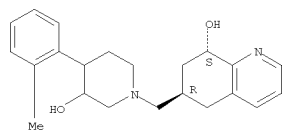
Absolute stereochemistry.



IT 1039359-51-7P 1039359-53-9P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic
preparation); BIOL (Biological study); PREP (Preparation)
(lipophilicity; synthesis and biol. evaluation of
arylpipecidinylmethyl-substituted cycloalkano[b]pyridines as orally
active opioid receptor-like 1 antagonists with minimal binding
affinity
to the hERG K⁺ channel)
RN 1039359-51-7 CAPLUS
CN 8-Quinololinol, 5,6,7,8-tetrahydro-6-[[3-hydroxy-4-(2-methylphenyl)-1-
piperidinyl]methyl]-, (6R,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1)
(CA INDEX NAME)

CM 1
CRN 1039359-50-6
CMF C22 H28 N2 O2

Absolute stereochemistry.



CM 2
CRN 87-69-4
CMF C4 H6 O6

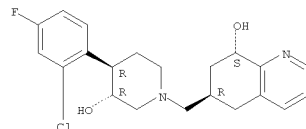
Absolute stereochemistry.

L13 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
arylpipecidinylmethyl-substituted cycloalkano[b]pyridines as orally
active opioid receptor-like 1 antagonists with minimal binding

affinity
to the hERG K⁺ channel)

RN 864828-68-2 CAPLUS
CN 8-Quinololinol, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-
piperidinyl]methyl]-5,6,7,8-tetrahydro-, hydrochloride (1:1), (6R,8S)-
(CA INDEX NAME)

Absolute stereochemistry.



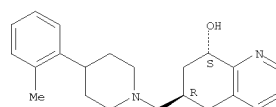
● HCl

IT 1039359-49-3P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic
preparation); BIOL (Biological study); PREP (Preparation)
(lipophilicity and acidity; synthesis and biol. evaluation of
arylpipecidinylmethyl-substituted cycloalkano[b]pyridines as orally
active opioid receptor-like 1 antagonists with minimal binding
affinity
to the hERG K⁺ channel)

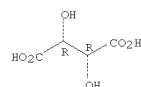
RN 1039359-49-3 CAPLUS
CN 8-Quinololinol, 5,6,7,8-tetrahydro-6-[[4-(2-methylphenyl)-1-
piperidinyl]methyl]-, (6R,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1)
(CA INDEX NAME)

CM 1
CRN 1039359-48-2
CMF C22 H28 N2 O

Absolute stereochemistry. Rotation (-).



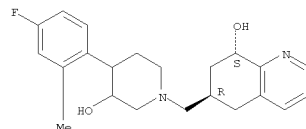
L13 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 1039359-53-9 CAPLUS
CN 8-Quinololinol, 6-[[4-(4-fluoro-2-methylphenyl)-3-hydroxy-1-
piperidinyl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)-,
(2R,3R)-2,3-dihydroxybutanedioate (1:1) (CA INDEX NAME)

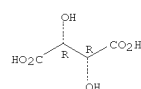
CM 1
CRN 1039359-52-8
CMF C22 H27 F N2 O2

Absolute stereochemistry.



CM 2
CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.



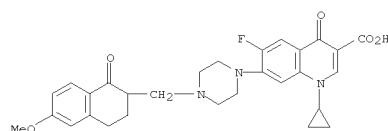
10590585.trn

L13 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN
 2008:670939 Document No. 149:100450 Synthesis of quinoline derivatives with
 antibacterial activity. Srivastava, Brijesh K.; Jain, Mukul R.; Patel,
 Pankaj R. (Cadila Healthcare Limited, India). Eur. Pat. Appl. EP 1927589
 A1 20080604, 19pp. DESIGNATED STATES: R: AT, BE, BG, CH, CY, CZ, DE,
 DK,
 EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, PL,
 PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, RS. (English). CODEN: EPXXDW.
 APPLICATION: EP 2007-254643 20071130. PRIORITY: IN 2006-MU1967 20061130.
 GI

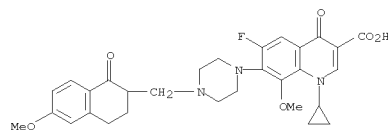
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention relates to a process for preparing quinoline
 compds. I
 [R1 = H, (C1-C12)alkyl, (C3-C12)cycloalkyl; R2, R3 = H, OH, halo, alkoxy,
 NO2, cyano; R8, R9, R10, R11 = H, alkyl; R4, R5, R6, R7 = H, halo,
 haloalkyl, OH, alkoxy, thio NO2, cyano, amino, (C1-C12)alkyl,
 (C1-C12)alkoxy derivative of sulfenyl or sulfonyl group, sulfonic acid
 and
 derivs.; Z = O, S, NR, R = H, OH, (C1-C3)alkyl; X = absent or CH2, O, S,
 SO, SO2; Y = (CH2)n, n = 0-3], their tautomeric forms, their
 pharmaceutically acceptable salts and pharmaceutical compns. containing
 them.
 For example, reacting 6-methoxy- α -tetralone with quinolinecarboxylic
 acid II gave piperazinyl quinoline III in 75% yield. Compound III and
 analog IV were tested for antibacterial activity; their pharmacokinetic
 profile was also explored.
 IT 1029844-02-7P, 1-Cyclopropyl-6-fluoro-7-[4-[(6-methoxy-1-oxo-
 1,2,3,4-tetrahydronaphthalen-2-yl)methyl]piperazin-1-yl]-4-oxo-1,4-
 dihydroquinoline-3-carboxylic acid
 RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); RCT
 (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL
 (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES
 (Uses)
 (preparation of (oxoquinolinyl)piperazine derivs. and their
 antibacterial
 activity)
 RN 1029844-02-7 CAPLUS
 CN 3-Quinolinecarboxylic acid,
 1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-[4-
 [(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-piperazinyl]-
 (CA INDEX NAME)

L13 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

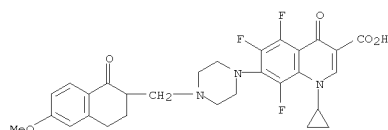


IT 1029844-04-9P, 1-Cyclopropyl-6-fluoro-8-methoxy-7-[4-[(6-methoxy-
 1-oxo-1,2,3,4-tetrahydronaphthalen-2-yl)methyl]piperazin-1-yl]-4-oxo-1,4-
 dihydroquinoline-3-carboxylic acid 1029844-05-0P,
 1-Cyclopropyl-5,6,8-trifluoro-7-[4-[(6-methoxy-1-oxo-1,2,3,4-
 tetrahydronaphthalen-2-yl)methyl]piperazin-1-yl]-4-oxo-1,4-
 dihydroquinoline-3-carboxylic acid 1029844-06-1P,
 1-Cyclopropyl-6-fluoro-8-methoxy-7-[4-[(6-methoxy-1-oxo-1,2,3,4-
 tetrahydronaphthalen-2-yl)methyl]-3-methylpiperazin-1-yl]-4-oxo-1,4-
 dihydroquinoline-3-carboxylic acid 1029844-07-2P,
 1-Ethyl-6-fluoro-7-[4-[(6-methoxy-1-oxo-1,2,3,4-tetrahydronaphthalen-2-
 yl)methyl]piperazin-1-yl]-4-oxo-1,4-dihydroquinoline-3-carboxylic acid
 1029844-18-5P, 1-Cyclopropyl-6-fluoro-7-[4-[(1-hydroxyimino-6-
 methoxy-1,2,3,4-tetrahydronaphthalen-2-yl)methyl]piperazin-1-yl]-4-oxo-1,4-
 dihydroquinoline-3-carboxylic acid
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (preparation of (oxoquinolinyl)piperazine derivs. and their
 antibacterial
 activity)
 RN 1029844-04-9 CAPLUS
 CN 3-Quinolinecarboxylic acid,
 1-cyclopropyl-6-fluoro-1,4-dihydro-8-methoxy-4-
 oxo-7-[4-[(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-
 piperazinyl]- (CA INDEX NAME)

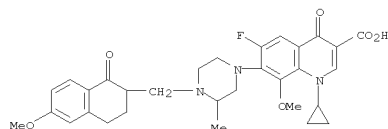


RN 1029844-05-0 CAPLUS
 CN 3-Quinolinecarboxylic acid, 1-cyclopropyl-5,6,8-trifluoro-1,4-dihydro-4-
 oxo-7-[4-[(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-
 piperazinyl]- (CA INDEX NAME)

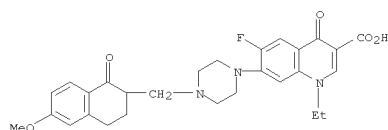
L13 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



RN 1029844-06-1 CAPLUS
 CN 3-Quinolinecarboxylic acid,
 1-cyclopropyl-6-fluoro-1,4-dihydro-8-methoxy-7-
 [3-methyl-4-[(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-
 piperazinyl]-4-oxo- (CA INDEX NAME)

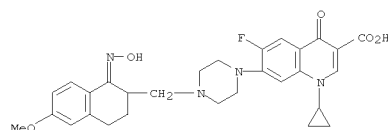


RN 1029844-07-2 CAPLUS
 CN 3-Quinolinecarboxylic acid, 1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-[4-
 [(1,2,3,4-tetrahydro-6-methoxy-1-oxo-2-naphthalenyl)methyl]-1-piperazinyl]-
 (CA INDEX NAME)



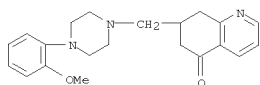
RN 1029844-18-5 CAPLUS
 CN 3-Quinolinecarboxylic acid,
 1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-[4-
 [(1,2,3,4-tetrahydro-1-(hydroxyimino)-6-methoxy-2-naphthalenyl)methyl]-1-
 piperazinyl]- (CA INDEX NAME)

L13 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



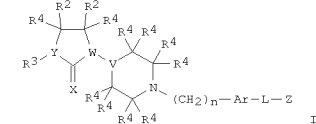
10590585.trn

L13 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN
 2007:655407 Document No. 147:2498640 Multistucture 3D-QSAR Studies on a Series of Conformationally Constrained Butyrophenones Docked into a New Homology Model of the 5-HT_{2A} Receptor. Dezi, Cristina; Brea, Jose; Alvarado, Mario; Ravina, Enrique; Masaguer, Christian F.; Loza, Maria Isabel; Sanz, Ferran; Pastor, Manuel (Research Unit on Biomedical Informatics (GRIB), IMIM, Universitat Pompeu Fabra, Barcelona, E-08003, Spain). Journal of Medicinal Chemistry, 50(14), 3242-3255 (English)
 2007: CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 147:249864. Publisher: American Chemical Society.
 AB The present study is part of a long-term research project aiming to gain insight into the mechanism of action of atypical antipsychotics. Here we describe a 3D-QSAR study carried out on a series of butyrophenones with affinity for the serotonin-2A receptor, aligned by docking into the binding site of a receptor model. The series studied has two peculiarities: (i) all the compds. have a chiral center and can be represented by two enantiomeric structures, and (ii) many of the structures can bind the receptor in two alternative orientations, posing the problem of how to select a single representative structure for every compound. We have used an original solution consisting of the simultaneous use of multiple structures, representing different configurations, binding conformations, and positions. The final model showed good statistical quality (n = 426, r₂ = 0.84, q₂LOO = 0.81) and its interpretation provided useful information, not obtainable from the simple inspection of the ligand-receptor complexes.
 IT 325489-07-4 325489-08-5 325489-09-6
 RL: PAC (Pharmacological activity); BIOL (Biological study) (multistucture QSAR studies on conformationally constrained butyrophenones docked into homol. model of 5-HT_{2A} receptor)
 RN 325489-07-4 CAPLUS
 CN 5(6H)-Quinolinone, 7-[[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



RN 325489-08-5 CAPLUS
 CN 5(6H)-Quinolinone, 7-[[[4-(4-fluorobenzoyl)-1-piperidinyl]methyl]-7,8-dihydro- (CA INDEX NAME)

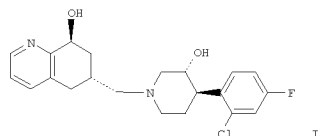
L13 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN
 2007:201033 Document No. 146:2743470 Substituted imidazolidinones and related compounds as chemokine receptor binding compounds and their preparation, pharmaceutical compositions and use in the treatment of infection of target cells by human immunodeficiency virus. Zhou, Yuanxi; Bourque, Elyse; Zhu, Yongbao; McEachern, Ernest J.; Harwig, Curtis; Skerlj, Renato T.; Bridger, Gary J.; Li, Tong-Shuang; Metz, Markus (Anomed Inc., Can.). PCT Int. Appl. WO 2007022371 A2 20070222, 363 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IS, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PTKXD2. APPLICATION: WO 2006-US32170 20060816. PRIORITY: US 2005-708471P 20050816.
 GI



10590585.trn

L13 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN
2006:941104 Document No. 145:335937 Preparation of A-form crystals of tetrahydroquinoline derivative and their medical compositions and pharmaceuticals. Sugimoto, Yuichi; Miyazoe, Hiroshi; Tsujita, Tomohiro (Banyu Pharmaceutical Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2006241096 A 20060914, 16pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2005-60632 20050304.

GI



I

AB A-form crystals of I.HCl are useful for prophylactic or therapeutic treatment of nociceptin receptor-associated diseases, e.g., pain, obesity, impaired learning, dementia, schizophrenia, depression, etc. Thus, trimethylsilylated I was deprotected, converted into HCl salt in MeOH, the solvent evaporated, dissolved in EtOH and treated with n-heptane to give A-form crystals of I.HCl, which inhibited the binding of [125I]-Tyr14-nociceptin to its receptor with IC50 value of 9.00 nM. The ray powder diffraction pattern of the crystals is also described.

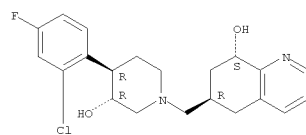
IT 864828-68-2P
RI: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of A-form crystals of tetrahydroquinoline derivative as nociceptin receptor antagonist)

RN 864828-68-2 CAPLUS
CN 8-Quinololinol, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-piperidinyl]methyl]-5,6,7,8-tetrahydro-, hydrochloride (1:1), (6R,8S)- (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

L13 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

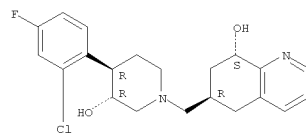


● HCl

IT 864830-99-9P 909781-64-2P
RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of A-form crystals of tetrahydroquinoline derivative as nociceptin receptor antagonist)

RN 864830-99-9 CAPLUS
CN 8-Quinololinol, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-piperidinyl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)- (CA INDEX NAME)

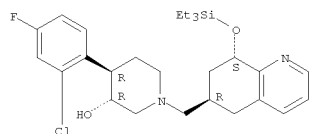
Absolute stereochemistry.



RN 909781-64-2 CAPLUS
CN 3-Piperidinol, 4-(2-chloro-4-fluorophenyl)-1-[[[(6R,8S)-5,6,7,8-tetrahydro-8-[(triethylsilyl)oxy]-6-quinolinyl]methyl]-, (3R,4R)- (CA INDEX NAME)

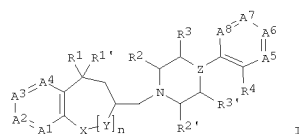
Absolute stereochemistry.

L13 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

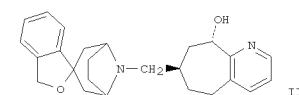


L13 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN
2005:1004733 Document No. 143:3061610 Preparation of cycloalkanopyridine derivatives as antagonists of nociceptin receptor. Takahashi, Hirobumi; Sugimoto, Yuichi; Yoshizumi, Takashi; Kato, Tetsuya; Asai, Masanori; Miyazoe, Hiroshi (Banyu Pharmaceutical Co., Ltd., Japan). PCT Int. Appl. WO 2005085228 A1 20050915, 205 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GB, GR, IE, IS, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, (Japanese). CODEN: PIXXD2. APPLICATION: WO 2005-JP4264 20050304. PRIORITY: JP 2004-62405 20040305.

GI



I



II

AB Cycloalkanopyridine derivs. represented by the general formula (I) [A1-A8 = (un)substituted CH or N, provided that at least one of A1-A4 is N; R1, R1' = H, halo, OH, cyano, Cl-6 alkyloxy, Cl-6 alkyloxyalkyloxy, Cl-6 alkyloxycarbonyl, Cl-6 alkyloxycarbonylamino, Cl-6 alkylcarbonyl, Cl-6 alkylcarbonyloxy, Cl-6 alkylcarbonylamino, Cl-6 alkylsulfonyl, etc.; or

R1 and R1' together form oxo or Cl-3 alkylene ketal; R2, R2' = H, Cl-6 alkyl, Cl-6 hydroxyalkyl or R2 and R2' or R3' together form Cl-3 alkylene or oxy-Cl-3 alkylene; R2' and R2 or R3 together form Cl-3 alkylene or oxy-Cl-3 alkylene; R3, R3' = H, HO, halo, Cl-6 alkyloxy, Cl-6 alkylcarbonyl, Cl-6 alkyloxycarbonyl, Cl-6 alkylsulfonyl, Cl-6 alkylsulfonylamino, Cl-6 alkylsulfonylalkylamino, cyano, (un)substituted Cl-6 alkyl; or R3 and R3' or R2' form Cl-3 alkylene or oxy-Cl-3 alkylene; or R3' and R3 or R2 together form Cl-3 alkylene or oxy-Cl-3 alkylene; R4 = H, halo, Cl-6 alkyl, Cl-6 hydroxyalkyl, Cl-6 haloalkyl, Cl-6 alkyloxy-Cl-6 alkyl, Cl-6 alkylcarbonyl, cyano, CHO, Cl-6 alkyloxycarbonyl, Cl-6 alkylcarbonylamino, Cl-6 alkyloxycarbonyl, etc.; X = CH2, CH(OH),

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L13 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
(un)substituted NH, O, S, SO₂; Y = CH₂, (un)substituted NH; Z = (un)substituted CH, N; N = 0,1] or pharmaceutically acceptable salts thereof are prepd. These compds. are nociceptin receptor antagonists and useful for treatment or prevention of diseases in which a nociceptin receptor participates, e.g. (1) as drugs for overcoming resistance to narcotic analgesics, (2) as analgesic enhancers, antiobesity agents, and appetite regulators, (3) as drugs for improving or preventing learning or memory decline or dementia in aging, cerebral vascular disorders, or Alzheimer's disease, (4) as cognition enhancers in attention deficit hyperactivity disorder or learning disorder during developmental stage, (5) as drugs for treatment of schizophrenia, (6) as drugs for treatment

of regressive neurodegenerative diseases such as Parkinson's disease and chorea, (6) as antidepressants or mood regulators, (7) as preventives or remedies for diabetes insipidus or polyuria, and (8) as remedies for hypotension. Thus, a soln. of 70 mg toluene-4-sulfonic acid [(7R,9S)-9-(tert-butylidimethylsilyloxy)-6,7,8,9-tetrahydro-5H-cyclohepta[b]pyridin-7-yl)methyl ester and 33 mg spiro[8-azabicyclo[3.2.1]octane-3,1'-3'H-isobenzofuran] hydrochloride in 1.0 mL N-methylpyrrolidone were treated with 124 mg NaI and 0.21 mL Et₃N and heated at 90° for 5 h with stirring, followed by treatment of the product with 1 M Bu₄NF/THF at 50° for 4 h and sepn. of the resulting racemate using chiral column (CHRALPAC AD column), to give (7R,9S)- and (7S,9R)-7-[spiro[8-azabicyclo[3.2.1]octane-3,1'-3'H-

isobenzofuran]-8-ylmethyl]-6,7,8,9-tetrahydro-5H-cyclohepta[b]pyridin-9-ol (II) and its (7R,9S)-stereoisomer. II inhibited the binding of [125I]Tyr¹⁴-nociceptin to human nociceptin receptor by 50% at 0.39 nM.

IT 864828-44-4P 864828-45-5P 864828-56-8P
864828-57-9P 864828-63-7P 864828-68-2P
864828-72-8P 864829-28-7P 864829-30-1P
864829-31-2P 864830-99-9P 864861-83-6P
864861-84-7P 864861-85-8P 864861-86-9P

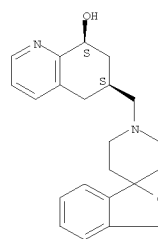
RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of cycloalkanopyridine derivs. as antagonists of nociceptin receptor for treating or preventing nociceptin receptor-associated diseases)

RN 864828-44-4 CAPLUS
CN 8-Quinololinol, 5,6,7,8-tetrahydro-6-(spiro[isobenzofuran-1(3H),4'-piperidin]-1'-ylmethyl)-, (6S,8S)- (CA INDEX NAME)

Absolute stereochemistry.

L13 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

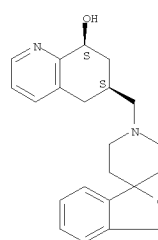


RN 864828-45-5 CAPLUS
CN 8-Quinololinol, 5,6,7,8-tetrahydro-6-(spiro[isobenzofuran-1(3H),4'-piperidin]-1'-ylmethyl)-, (6S,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 864828-44-4
CMF C22 H26 N2 O2

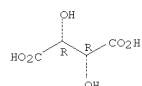
Absolute stereochemistry.



CM 2

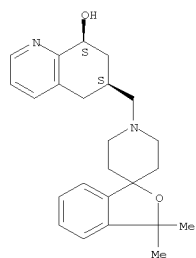
L13 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.



RN 864828-56-8 CAPLUS
CN 8-Quinololinol, 6-[[3,3-dimethylspiro[isobenzofuran-1(3H),4'-piperidin]-1'-yl)methyl]-5,6,7,8-tetrahydro-, (6S,8S)- (CA INDEX NAME)

Absolute stereochemistry.



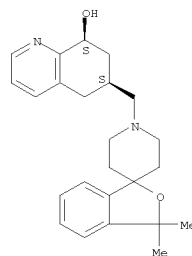
RN 864828-57-9 CAPLUS
CN 8-Quinololinol, 6-[[3,3-dimethylspiro[isobenzofuran-1(3H),4'-piperidin]-1'-yl)methyl]-5,6,7,8-tetrahydro-, (6S,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 864828-56-8
CMF C24 H30 N2 O2

Absolute stereochemistry.

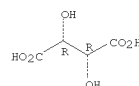
L13 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 2

CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.

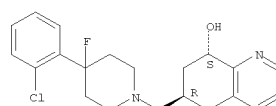


RN 864828-63-7 CAPLUS
CN 8-Quinololinol, 6-[[4-(2-chlorophenyl)-4-fluoro-1-piperidinyl)methyl]-5,6,7,8-tetrahydro-, (6R,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 864828-62-6
CMF C21 H24 Cl F N2 O

Absolute stereochemistry.



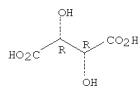
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L13 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

CM 2

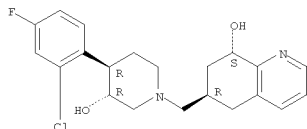
CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.



RN 864828-68-2 CAPLUS
CN 8-Quinololinol, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-piperidinyl]methyl]-5,6,7,8-tetrahydro-, hydrochloride (1:1), (6R,8S)- (CA INDEX NAME)

Absolute stereochemistry.



● HCl

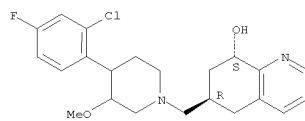
RN 864828-72-8 CAPLUS
CN 8-Quinololinol, 6-[[[4-(2-chloro-4-fluorophenyl)-3-methoxy-1-piperidinyl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 864828-71-7
CMF C22 H26 Cl F N2 O2

Absolute stereochemistry.

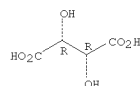
L13 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 2

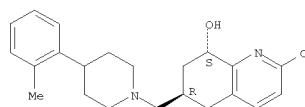
CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.



RN 864829-28-7 CAPLUS
CN 8-Quinololinol, 2-chloro-5,6,7,8-tetrahydro-6-[[4-(2-methylphenyl)-1-piperidinyl]methyl]-, (6R,8S)-rel- (CA INDEX NAME)

Relative stereochemistry.



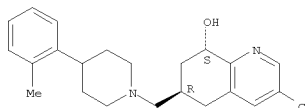
RN 864829-30-1 CAPLUS
CN 8-Quinololinol, 3-chloro-5,6,7,8-tetrahydro-6-[[4-(2-methylphenyl)-1-piperidinyl]methyl]-, (6R,8S)-rel-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 864829-29-8
CMF C22 H27 Cl N2 O

Relative stereochemistry.

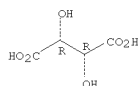
L13 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)



CM 2

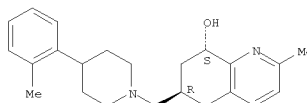
CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.



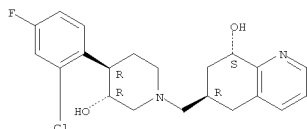
RN 864829-31-2 CAPLUS
CN 8-Quinololinol, 5,6,7,8-tetrahydro-2-methyl-6-[[4-(2-methylphenyl)-1-piperidinyl]methyl]-, (6R,8S)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 864830-99-9 CAPLUS
CN 8-Quinololinol, 6-[[[(3R,4R)-4-(2-chloro-4-fluorophenyl)-3-hydroxy-1-piperidinyl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)- (CA INDEX NAME)

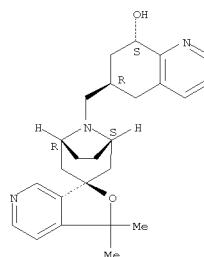
Absolute stereochemistry.



L13 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

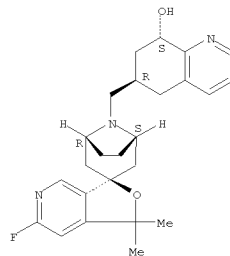
RN 864861-83-6 CAPLUS
CN 8-Quinololinol, 6-[[[1',1'-dimethylspiro[(3-endo)-8-azabicyclo[3.2.1]octane-3,3'(1'H)-furo[3,4-c]pyridin]-8-yl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 864861-84-7 CAPLUS
CN 8-Quinololinol, 6-[[[6'-fluoro-1',1'-dimethylspiro[(3-endo)-8-azabicyclo[3.2.1]octane-3,3'(1'H)-furo[3,4-c]pyridin]-8-yl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 864861-85-8 CAPLUS
CN 8-Quinololinol, 6-[[[(1R,5S)-6'-fluoro-1',1'-dimethylspiro[8-azabicyclo[3.2.1]octane-3,3'(1'H)-furo[3,4-c]pyridin]-8-yl]methyl]-5,6,7,8-tetrahydro-, (6R,8S)- (CA INDEX NAME)

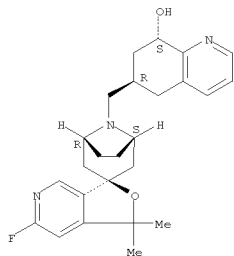
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L13 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)
tetrahydro-, (6R,8S)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (salt)
(9CI) (CA INDEX NAME)

CM 1

CRN 864861-84-7
CMP C25 H30 F N3 O2

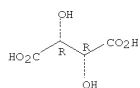
Absolute stereochemistry.



CM 2

CRN 87-69-4
CMP C4 H6 O6

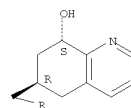
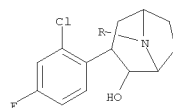
Absolute stereochemistry.



RN 864861-86-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-2-ol, 3-(2-chloro-4-fluorophenyl)-8-[[[(6R,8S)-5,6,7,8-tetrahydro-8-hydroxy-6-quinolinyl]methyl]-, hydrochloride (1:1)
(CA INDEX NAME)

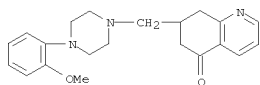
Absolute stereochemistry.

L13 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN (Continued)

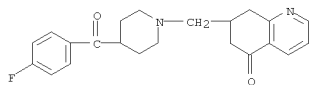


● HCl

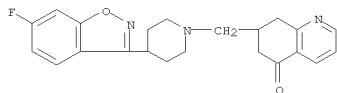
L13 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2010 ACS on STN
2000:855012 Document No. 134:1629040 A simple, efficient method for regioselective synthesis of 7-aminomethyl-7,8-dihydro-6H-quinolin-5-ones, new potential CNS agents. Pita, B.; Masaguer, C. F.; Ravina, E.
(Facultad de Farmacia, Laboratorio de Química Farmacéutica, Departamento de Química Orgánica, Universidad de Santiago de Compostela, Santiago de Compostela, 15706, Spain). Tetrahedron Letters, 41(50), 9829-9833 (English) 2000.
CODEN: TELEAY. ISSN: 0040-4039. OTHER SOURCES: CASREACT 134:162904.
Publisher: Elsevier Science Ltd..
AB An efficient and convenient strategy for the regioselective synthesis of new conformationally restricted butyrophenones of the quinoline series is presented. 7-(Aminomethyl)-7,8-dihydro-6H-quinolin-5-ones were obtained from 7-(methoxymethyl)-7,8-dihydro-6H-quinolin-5-one via the tosylate, and also in a 1-pot reaction via 7-(bromomethyl)-7,8-dihydro-6H-quinolin-5-one, with moderate-to-good overall yields in both cases.
IT 325489-07-4P 325489-08-5P 325489-09-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (aminomethyl)dihydroquinolinones)
RN 325489-07-4 CAPLUS
CN 5(6H)-Quinolinone, 7-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



RN 325489-08-5 CAPLUS
CN 5(6H)-Quinolinone, 7-[[4-(4-fluorobenzoyl)-1-piperidinyl]methyl]-7,8-dihydro- (CA INDEX NAME)



RN 325489-09-6 CAPLUS
CN 5(6H)-Quinolinone, 7-[[4-(6-fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]methyl]-7,8-dihydro- (CA INDEX NAME)



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